Lawrence Livermore National Laboratory

# Science & Technology Review

April/May 2015


## Science-Based Disaster Response

*Also in this issue:*

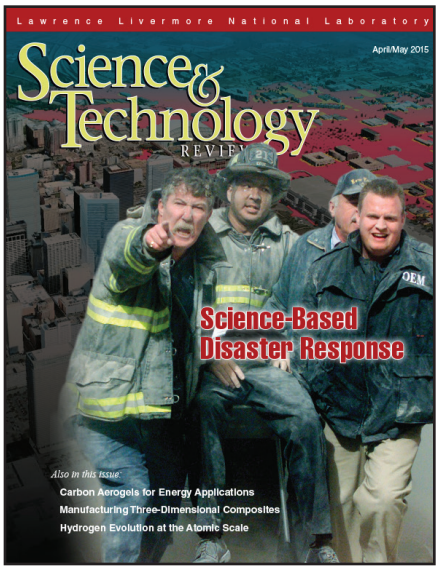
**Carbon Aerogels for Energy Applications**

**Manufacturing Three-Dimensional Composites**

**Hydrogen Evolution at the Atomic Scale**

## About the Cover

Lawrence Livermore researchers are working with federal agencies to help cities better prepare for the critical minutes and hours following a natural or human-caused disaster. Advanced modeling and simulations reveal that science-based planning is key to saving tens of thousands of lives. As the article on p. 4 describes, the Laboratory is assisting the Federal Emergency Management Agency and other Department of Homeland Security agencies to further the science-based understanding of what to expect from detonation of an improvised nuclear device or dispersal of a toxic chemical. On the cover, a group of first responders is superimposed on a Livermore simulation of a chlorine gas spill (red) near downtown Houston, Texas. (Responder photo courtesy of Rueters/Shannon Stapleton.)

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## About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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April/May 2015

Lawrence Livermore National Laboratory

# Contents

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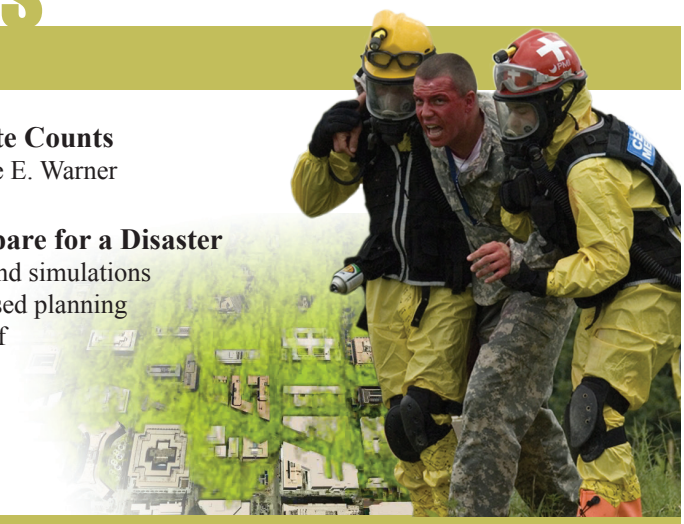
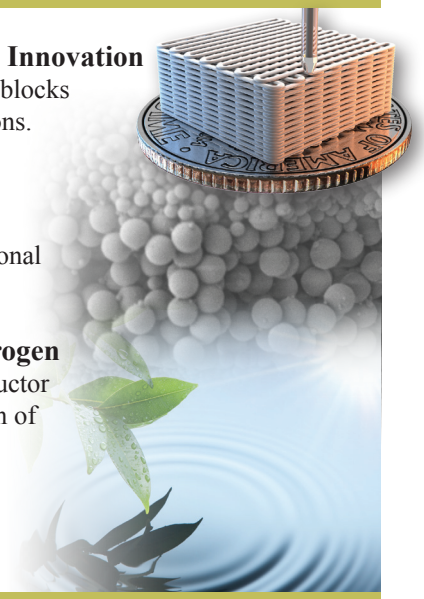
## Feature



3 **When Every Minute Counts**
Commentary by Bruce E. Warner

4 **Helping Cities Prepare for a Disaster**
Advanced modeling and simulations reveal that science-based planning is key to saving tens of thousands of lives.

## Research Highlights



14 **Energy Applications Drive Carbon Aerogel Innovation**
Newer forms of carbon are providing the building blocks for a range of energy and environmental applications.

19 **A Guiding Light for Designer Materials**
Light-directed electrophoretic deposition uses photoconductive electrodes to build three-dimensional multimaterial composites.

23 **Diving into the Dynamics of Evolving Hydrogen**
Simulations of how sunlight, water, and semiconductor materials interact provide insights on the formation of hydrogen fuel.

## Departments

2 The Laboratory in the News

27 Patents and Awards

29 Abstract

## Microcapsules Capture Carbon Safely

Lawrence Livermore scientists, along with colleagues from Harvard University and the University of Illinois at Urbana-Champaign, have developed a new type of carbon capture media composed of core-shell microcapsules. Each capsule consists of a highly permeable polymer shell and a fluid (sodium carbonate solution) that reacts with and absorbs carbon dioxide ($CO_2$). The capsules keep the liquid contained inside the core and allow the $CO_2$ gas to pass back and forth through the capsule shell. The team's work was published online in the February 5, 2015, edition of *Nature Communications*.

The aim of carbon capture is to prevent the release of large quantities of $CO_2$—a greenhouse gas that traps heat and makes the planet warmer—into the atmosphere from fossil fuel use in power generation and other industries. However, currently used carbon capture methods can be harmful to the environment. "Our method is a huge improvement in terms of environmental impacts because we are able to use simple baking soda, present in every kitchen, as the active chemical for capturing $CO_2$," says Roger Aines, one of the Lawrence Livermore team members.

The ability to move away from caustic fluids, such as monoethanolamine, to more environmentally benign ones, such as carbonates, is a key attribute of the team's research. Unlike the more caustic sorbents, the microcapsules react only with the gas of interest (in this case $CO_2$). The new process can be designed to work with coal or natural gas-fired power plants as well as in industrial processes such as steel and cement production. "The microcapsule technology provides a a more efficient method for carbon capture with fewer environmental issues," says Aines.

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## Humans Accelerate Soil Erosion

Research published in the January 7, 2015, online edition of *Geology* reports that humans' use of land has eroded soil 100 times faster than natural processes. Scientists discovered that the rate of hillslope erosion before European settlement was about 2.5 centimeters every 2,500 years, but spiked to about 2.5 centimeters every 25 years because of increased logging and agriculture use in the late 1800s and early 1900s. "The Earth doesn't create that precious soil for crops fast enough to replenish what the humans took off," says former Laboratory scientist Dylan Rood, who conducted the research while at Livermore. "This pattern is unsustainable if continued."

The team, which also includes Lucas Reusser and Paul Bierman of the Rubenstein School of Environment and Natural Resources at the University of Vermont, collected 24 sediment samples from the Roanoke, Savannah, and Chattahoochee rivers along with seven other river basins, where clay soils were built up over many millennia. From these samples, the team extracted a rare isotope of beryllium, Be-10, which is formed by cosmic rays and builds up in about the top meter of soil. The slower the rate of erosion, the longer the soil is exposed at Earth's surface, and the more Be-10 the soil accumulates. Using Livermore's Center for Accelerator Mass Spectrometry, Rood measured how much Be-10 was in the samples, and found, for the first time, a precise quantification of this background rate of erosion. The background rates were then compared to postsettlement rates of both upland erosion and downriver sediment yield. Says Rood, "We can use the Be-10 erosion rates as a target for successful resource conservation strategies to develop smart environmental policies and regulations that will protect threatened soil and water resources for generations to come."

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## Peering into Cosmic Magnetic Fields

In a *Nature Physics* paper published on January 19, 2015, Lawrence Livermore researchers report, for the first time, well-developed, oriented magnetic filaments generated by the Weibel mechanism in counter-streaming, collisionless flows from high-power lasers. The team's findings demonstrate the power of the Weibel filamentation instability—a plasma instability present in homogeneous or nearly homogeneous electromagnetic plasmas—to produce small-scale seed magnetic fields throughout the cosmos. These fields can be further amplified to larger scales to create the ubiquitous magnetic fields that exist in astrophysical systems.

Experiments were conducted at the Omega Laser Facility at the University of Rochester's Laboratory for Laser Energetics. The researchers used protons produced by the implosion of a deuterium and helium capsule. The resulting data revealed the elusive Weibel filamentation instability. "A range of magnetic field scales exist in the cosmos, but the origin of these fields has been elusive," says lead author Channing Huntington, a Livermore physicist. "Weibel instability has long been theorized as a mechanism to generate these fields, but this work offers the most compelling experimental evidence to date that it is indeed possible."

The team envisions a broad range of follow-up experiments on Omega to test the magnetic field generation under conditions that are relevant to astrophysical systems. The researchers also have begun experiments at the Laboratory's National Ignition Facility, where larger, faster plasma flows could produce even higher fields and the Weibel-mediated shock formation would be fully mature. These experiments will reach conditions not previously achieved in a laboratory setting.

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Commentary by Bruce E. Warner

# When Every Minute Counts



FORMER U.S. Secretary of State George P. Shultz once said of the Laboratory, "Your mission is to make the nation safer." National security is our greatest responsibility, and through the years, we have applied innovative science and technology to address this challenge. Lawrence Livermore uses multidisciplinary capabilities, including in physical and life sciences, computation, and engineering, to reduce global threats and solve pressing national security problems. As part of this mission, we support the Department of Energy (DOE), the Department of Homeland Security, and the Federal Emergency Management Agency in preparing for disasters such as a chemical accident, a natural disaster, or a terrorist attack involving weapons of mass destruction (WMD).

The article beginning on p. 4 describes how Lawrence Livermore is applying its expertise in atmospheric modeling, WMD materials, and explosion dynamics to help first responders and community leaders prepare for emergencies, from a railcar chemical spill to a nuclear explosion in a U.S. city. Police, firefighters, emergency medical technicians, and city emergency response managers make crucial decisions in the first minutes to hours after a catastrophic event that affect how many lives can be saved. The Laboratory is providing the tools that first responders and city organizations need to make informed decisions. These tools consist of science-based emergency response plans, realistic training, and advanced computer models and simulations that show what can be expected during and after emergency situations.

Our models demonstrate the complexity of material and fallout plumes and how the transport and deposition of hazards change over time. With this information, the Laboratory helps first responders and state and local agencies develop contingency plans that can be as detailed as block-by-block guidance. We enthusiastically support these efforts, which may one day help save lives.

This issue of *Science & Technology Review* also includes three highlights that demonstrate how Laboratory researchers apply their expertise to develop novel materials and techniques to meet mission objectives. The research is conducted at the intersection of basic and applied science and as such provides vivid examples of how fundamental understanding of complex processes can lead to practical, beneficial applications. The highlight beginning on p. 14 describes recent advances in carbon aerogels that may be useful for a range of new energy and environmental purposes, including hydrogen storage, electrical energy storage, catalytic support in fuel cells, and desalination using capacitive deionization.

A new Laboratory-developed additive manufacturing (AM) technique that uses photoconductive electrodes to create three-dimensional multimaterial composites is discussed in the highlight beginning on p. 19. Building on traditional electrophoretic deposition (EPD) methods, the researchers involved in this effort have made advances in material flow and dynamic patterning to improve AM capabilities. Called light-directed EPD, this method shows promise for developing novel materials with unique properties, improving component quality, and significantly reducing associated production time and cost.

The final highlight, which begins on p. 23, describes Lawrence Livermore's simulation and modeling work on photoelectrochemical processes for producing hydrogen fuel, a DOE-sponsored project. Through their computational efforts, researchers are bolstering understanding of the complex atomic and molecular interactions of sunlight, water, and semiconductors in the hydrogen evolution process, which could provide a basis for cost-effective, efficient, and environmentally responsible solar-to-chemical energy conversion.

Together, these articles exemplify what a federally funded research and development center is meant to do: make scientific discoveries and technological advances that support our nation's needs, and in the case of Lawrence Livermore, ensure national security. The work has urgency and practicality and spans government agencies at the local, state, and federal levels. It shows our ability to respond to current challenges and anticipate future ones. Whether we are helping to provide communities with disaster preparedness plans or establishing ways to improve the nation's economic competitiveness, national security is always our end goal. At Livermore, we excel at research, development, and implementation because we understand that when it comes to saving lives and meeting national needs, every minute counts.

■ Bruce E. Warner is principal associate director for Global Security.

# Helping Cities PREPARE for a Disaster

*Researchers use advanced modeling and simulations to show how urban dwellers can survive both natural and human-caused events.*

FOR several decades, Lawrence Livermore researchers have helped federal emergency officials and their state and local counterparts to better understand the science underlying a host of natural and human-caused disasters. More recently, the Laboratory has been working to formulate the most effective ways for responding to low-probability, high-consequence human-caused events involving nuclear, chemical, or biological materials. This task has become more urgent as the nation's population continues to move into dense urban centers, where large numbers of people gather in public areas such as arenas.

"The federal government wants communities to better prepare for the critical minutes and hours shortly following a disaster," says Livermore's Amy Waters, program leader for Explosives and Infrastructure Security. Toward that end, Livermore researchers use advanced modeling and simulations to show that many lives can be saved during incidents that once seemed impossible for which to prepare, in particular for events that can occur without warning. Livermore simulations, shared broadly with federal, state, and local agencies nationwide, serve as excellent training tools and can form the basis for community-specific emergency response plans. Waters says, "Emergency response personnel need plans in place that are technically informed."

In particular, the Laboratory is assisting the Federal Emergency Management Agency (FEMA) and other Department of Homeland Security (DHS) agencies to further the science-based understanding of what to expect from detonation of an improvised nuclear device (IND) or dispersal of a toxic chemical. Waters notes that historically a disconnect has existed between researchers working to resolve scientific questions about the likely effect of, for example, a detonated IND and the practical needs of emergency responders. During such an event, responders would be working with incomplete information, under severe time pressure, and, very likely, in the midst of mass panic and confusion. The Livermore simulations are showing officials—and the public—what to prepare for in the first critical minutes and hours. The simulations demonstrate, for example, how dense urban landscapes can mitigate the effects of an IND and provide valuable protection from fallout.

"The most important message," says Waters, "is that many lives can be saved with appropriate planning and preparedness." She notes, however, that the findings from science-based planning may at first seem counterintuitive. For example, denser-than-air clouds of toxic gases can remain concentrated close to the surface, disperse upwind, or persist longer than expected when trapped in urban areas. Likewise, immediate evacuation may not be wise following the detonation of an IND because of the high levels of initial fallout radiation. Evacuation may also be difficult because of the likelihood of car crashes caused by the initial burst of blinding light and street blockages caused by blast-generated rubble.

The Laboratory has a long history of developing models that track the transport and deposition of hazardous materials released into the atmosphere, thanks in large part to the National Atmospheric Release Advisory Center (NARAC). This federal facility, located at Livermore, serves as the Department of Energy's (DOE's) plume-modeling center for real-time assessments of the impacts of nuclear, radiological, chemical, biological, or natural emissions. NARAC has responded to numerous emergencies over more than three decades, beginning with the Three Mile Island nuclear power plant incident in 1979.

NARAC simulations couple meteorological, geographical, and material property data with computer models that account for the physical processes affecting the dispersion and deposition of radioactive and other toxic materials. For example, fallout simulations can show the trajectory of the plume and how much material is deposited onto buildings and streets. Maps of fallout plumes and ground


concentrations inform disaster response plans and are valuable in training first responders on what to expect.

## Models Point the Way

In 2008, DHS's Office of Health Affairs (OHA) launched a program to identify scientific consensus and recommend actions that local emergency responders should take to prepare for an IND detonation in their city. A 10-kiloton IND (equivalent to energy produced by 10,000 metric tons of TNT) could kill tens of thousands of people, particularly if it were set off in a dense U.S. urban setting that lacked sound response plans. The OHA program addressed a directive from Congress, whose members were concerned that cities had insufficient guidance to prepare for acts of nuclear terrorism.

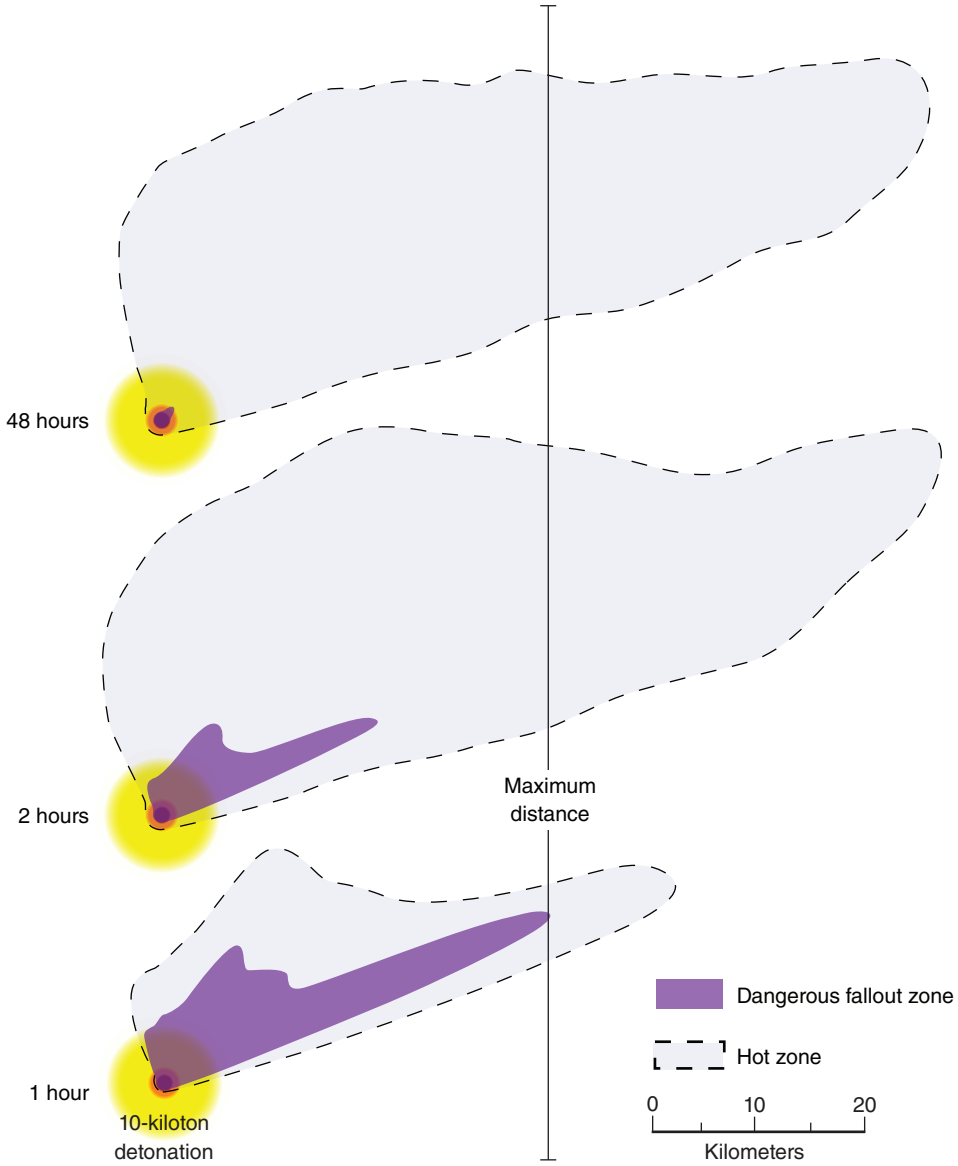
For the OHA effort, Livermore health physicist Brooke Buddemeier chaired a working group composed of experts from several federal agencies and DOE national laboratories. At the time, minimal research had been done on the likely effects and best mitigation strategies specific to a low-yield, ground-level detonation of an IND in a modern U.S. city. Concurrently, as part of an integrated terrorism assessment for DHS's Science and Technology Directorate, Buddemeier and colleagues had begun a multiagency effort to develop detailed public health and medical impact

assessments from the same type of event. Because of the large difference in destructive power between INDs and strategic thermonuclear weapons of the Cold War, much of the civil defense era guidance did not apply. Historic data from aboveground nuclear tests could be used for estimating the effects from an IND, but very few tests were conducted at ground level.

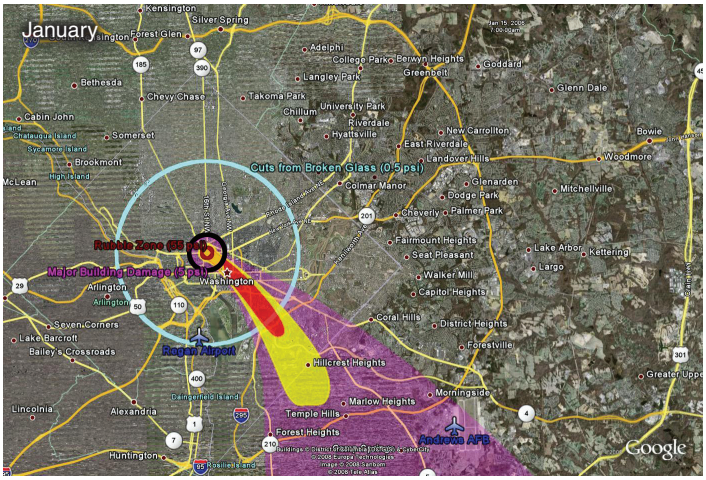
According to Buddemeier, perceptions among city planners have been shaped by Cold War thermonuclear attack scenarios. As a result, planning for an IND event has seemed overwhelming to agencies charged with public health and safety. Says Buddemeier, "Some people assume nothing can be done because 'we will all be dead,' or that a detonation response is 'a federal problem.' Unfortunately, such inattention in local planning could lead to tens of thousands of preventable casualties. When this effort began, a lack of scientific consensus existed regarding key protective measures such as shelter and evacuation."

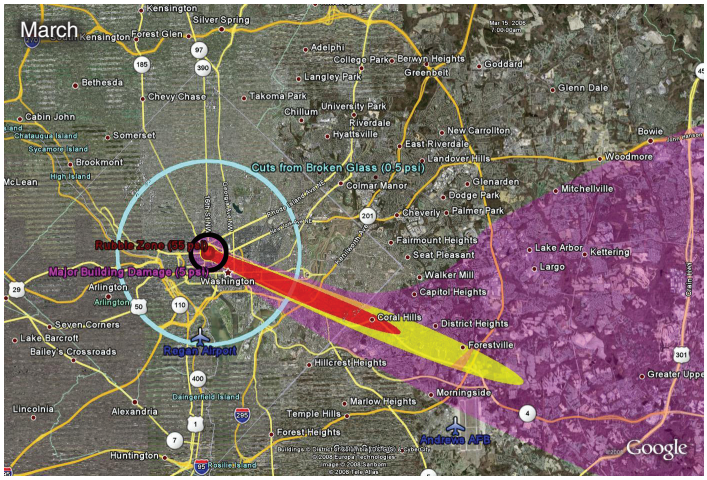
Buddemeier and colleagues reviewed a number of nuclear weapon effects studies. They also performed detailed modeling of the effects of a nuclear detonation in a number of U.S. cities, drawing on data from more than 1,000 Cold War nuclear tests and the experiences of Hiroshima and Nagasaki. The outcome of this effort was the 2009 Lawrence Livermore report, *Key Response Planning Factors for the Aftermath of Nuclear Terrorism*. The document recommends practical ways to plan for an IND and potentially prevent many fatalities and casualties. The Executive Office of the President also used this research to support the 2009 interagency document, *Planning Guidance for Response to a Nuclear Detonation*. This report, updated in 2010, continues to support preparedness documents and training materials for major U.S. cities. "Our most important responsibility is translating science into actionable information for responders and the public that will save lives," Buddemeier says. The OHA initiative continues today primarily under FEMA, which is working to strengthen regional IND response planning in all FEMA regions.

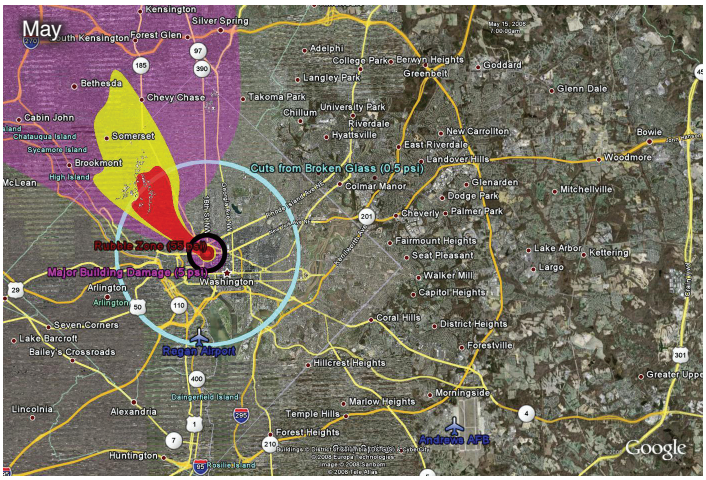
Mitigating the impacts of an IND requires understanding both prompt effects and delayed fallout. Prompt effects radiate through an area immediately following a detonation and could cause hundreds of thousands of casualties within a few

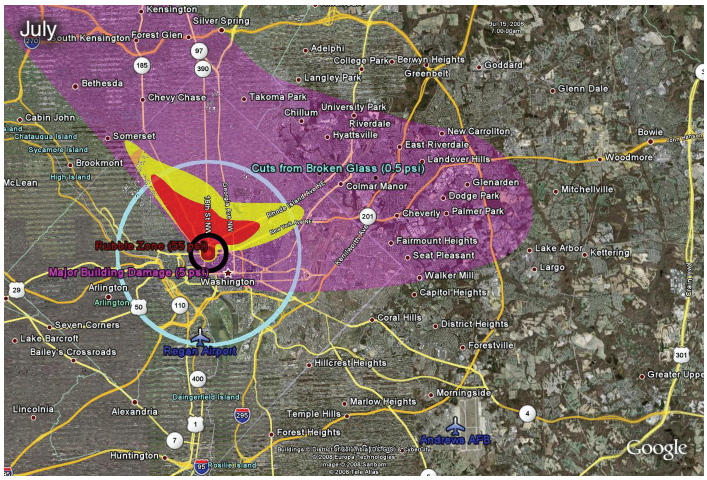


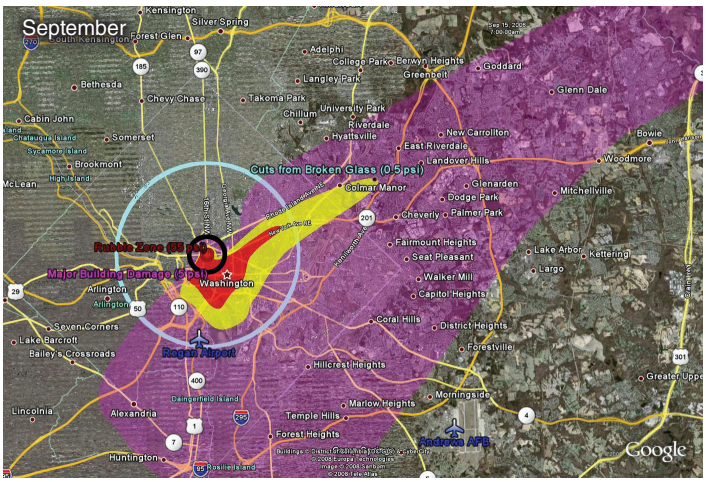

Prompt effects from a simulated 10-kiloton improvised nuclear device (IND) radiate immediately following a detonation. These effects include an intense flash of light, a shockwave, heat, and both ionizing and electromagnetic radiation. The dangerous fallout zone (radiation levels greater than 10 rems per hour) in purple shrinks quickly, while the much less dangerous hot zone (radiation level greater than 0.01 rems per hour) continues to grow for about 24 hours postdetonation as radioactive material is transported and deposited further downwind. (A rem is a unit of absorbed ionizing radiation. Doses greater than several hundred rem can be fatal.)

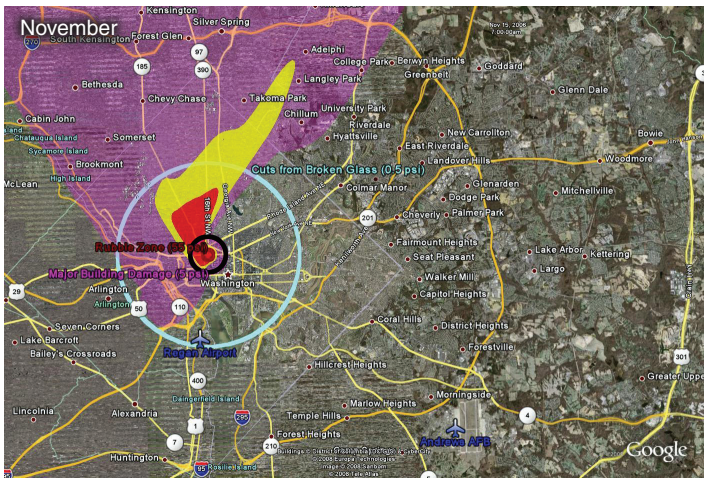



Simulations from the National Atmospheric Release Advisory Center reveal how changing weather over the greater Washington, DC, area can cause complex and variable fallout patterns. The weather data used for the simulations were obtained at noon on the 15th of each month in 2006 (six months are shown here). The inner black circle denotes major building damage, and the outer blue circle is the range where glass is broken with enough force to cause injury. The colors of the fallout areas represent 300 rems (red), 100 rems (yellow), and 1 rem (magenta) for a two-hour exposure period. (Images courtesy of Google.)

kilometers. These effects include an intense flash of light, a shockwave, heat, and both ionizing and electromagnetic radiation. The flash of light would likely temporarily blind anyone within 10 kilometers. As a result, most roads within this range would likely be clogged with accidents, which is an important planning factor.

Many previous modeling studies have overpredicted prompt effects in the urban environment because the models did not consider how urban buildings would mitigate some effects on the population. However, advanced radiation transport models show a significant reduction in the range of thermal and prompt radiation effects in urban areas.

Radioactive fallout is generated when the dust and debris excavated by the initial explosion combine with radioactive fission products produced in the nuclear detonation and then are drawn upward several kilometers. The highly radioactive particles can then drop to earth. Unlike prompt effects, which occur too rapidly to be easily avoided, exposure to fallout radiation can be minimized by proper action. Advanced Livermore shelter modeling has helped evaluate the extent to which typical urban buildings can protect citizens if people are provided with a few simple guidelines.

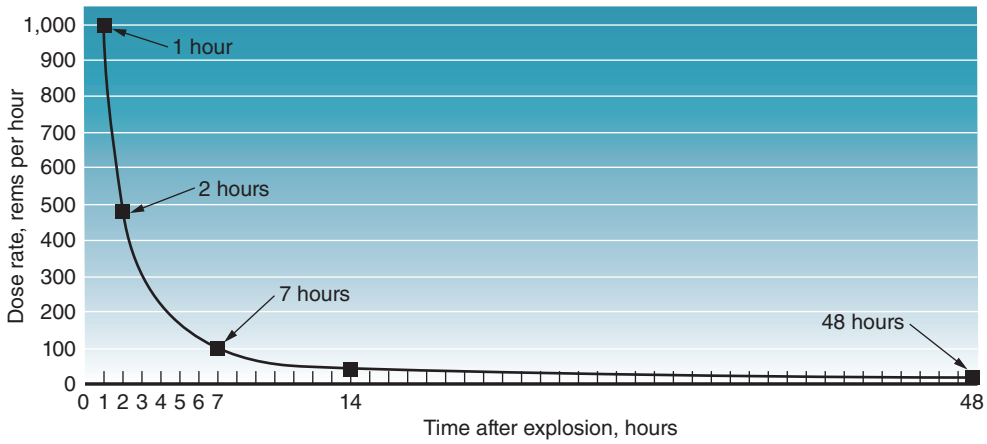
To inform FEMA regional response planning, Livermore researchers have made computer simulations showing prompt effects and fallout patterns from hypothetical INDs for a number of U.S. cities. Fallout modeling is performed with a suite of dispersion and meteorological computer codes, many of which have been developed at NARAC. The models incorporate real-world weather conditions, including wind speeds and direction at different locations and altitudes that are critical when calculating the transport and deposition of fallout. By incorporating advanced geospatial analysis and overlays generated in Google Earth, the simulations allow block-by-block analyses of prompt blast, thermal, and radiation effects, as well as fallout arrival and decay over time.

## Block-by-Block Analyses

"We've moved away from simple circles and cigar-shaped contour plots of prompt and integrated fallout exposures," says Buddemeier. "Now we divide a city into individual blocks and buildings and view events unfolding minute by minute based on an observed weather pattern for a chosen day and hour."

Livermore simulations reveal that the most important action following an IND detonation is to reduce fallout exposure with early adequate sheltering followed by delayed, informed evacuation. Fallout decays rapidly, releasing more than half its energy in the first hour because of the short half-lives of many radionuclides. The primary hazard from fallout is not from breathing in radioactive particles but from exposure to the particles that have settled on the ground and on roofs. Because people who are outdoors or inside vehicles will have little protection from fallout, they should move quickly into the nearest robust (concrete or brick) building—ideally, either below ground, such as in a basement or parking garage, or into the middle floors of a multistory building. "Our simulations show that nearly all fallout casualties can be eliminated by taking proper steps in the first few minutes and hours of the event," says Buddemeier.

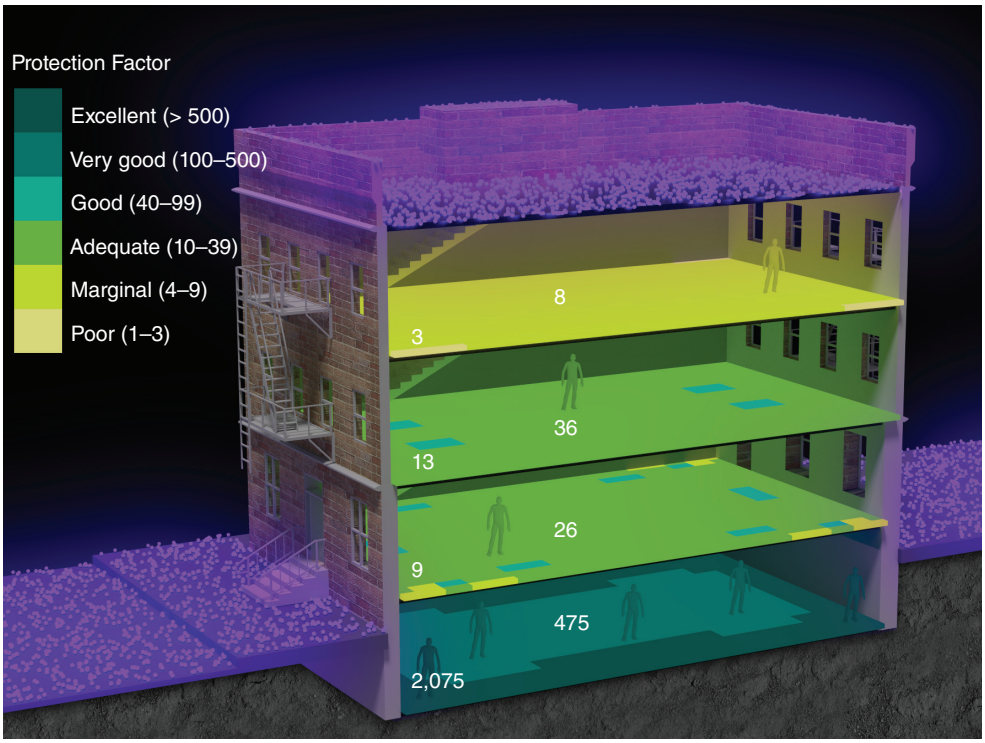
As a participant in FEMA-sponsored regional preparedness activities, Buddemeier has presented to local officials and emergency response personnel advanced simulations that compare the relative degrees of protection afforded by different types of buildings. His message is that science-based response plans can "save many lives in the first few hours." Common misconceptions about fallout are dispelled when people watch the simulated fallout cloud from an IND detonation moving across an urban area with radiation readings first growing and then shrinking. The simulations also show many nuances to sheltering in place followed by informed evacuation. For example, it is counterproductive for someone to evacuate when they do not have the information needed to avoid fallout areas. The advanced multimedia simulations produced by this effort help responders and planners understand "what they will see, what they will know, and the impact of their decisions," says Buddemeier.




Following an IND detonation, sheltering for the first few hours, when the radiation levels are highest, can help avoid significant evacuation exposures.

## Tracking Toxic Chemical Releases

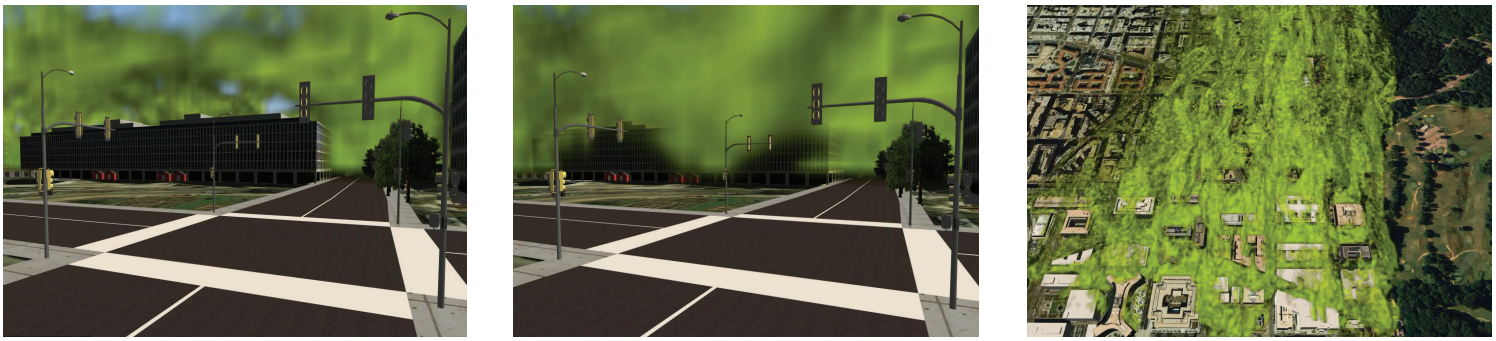
Livermore scientists are also supporting disaster response planning for the release of a toxic chemical, whether by terrorists or by accident. They consider a range of scenarios, based on examples ranging from the 2005 freight train derailment that released 60 tons of chlorine gas in Graniteville, South Carolina, to the 1995 Japanese cult's release of sarin nerve gas in the Tokyo subway system. Each city is unique, with its own set of factors that shape disaster response. For example, a city may have large venues where people gather, or a large concentration of chemical processing plants, or freight trains that regularly travel through carrying toxic chemicals.




Adequate shelters such as this brick apartment building can shield occupants from the penetrating radiation of radioactive fallout. The most protection is afforded in a basement away from exterior walls. The top floor offers the least protection because it is close to fallout accumulation on the roof. (Rendering by Ryan Chen.)

Livermore scientist Akshay Gowardhan is developing a NARAC code named Aeolus that simulates flow and dispersion in urban areas. Aeolus explicitly resolves individual buildings and can simulate the atmospheric dispersion of toxic gases and particles, including denser-than-air gases. The model has been validated against experimental data from urban field experiments with tracer gas releases.

Gowardhan explains that buildings influence the movement of gases, creating complicated and at times nonintuitive flow patterns. His code simulates complex airflow phenomena such as eddies that occur at street intersections and vertical drafts caused by skyscrapers. The code can be run in either a high-fidelity or fast-running model. While other building-resolving codes require a supercomputer, Aeolus runs on a laptop. Although it is currently being used for planning and



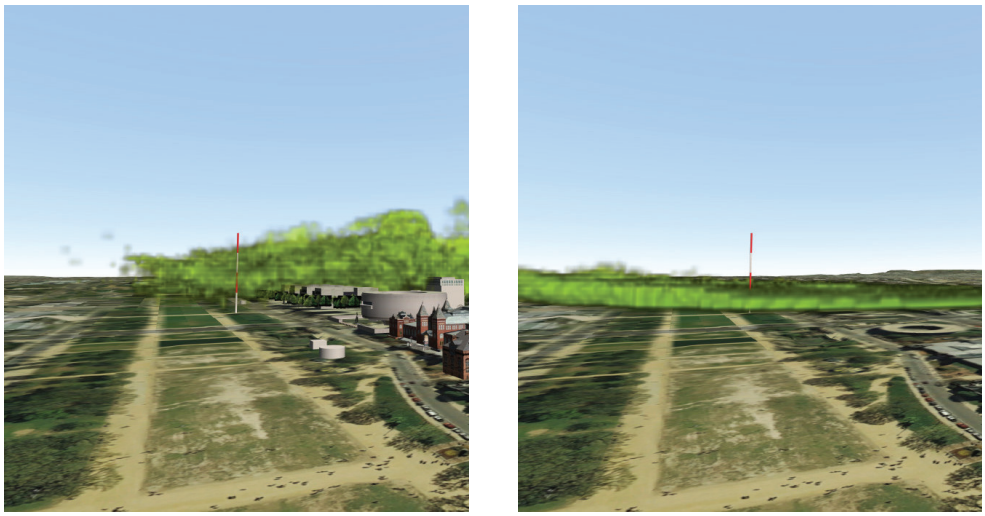
These visualizations of an Aeolus simulation, created using Livermore's SceneWorks software, depict the aftermath from a ruptured chlorine tank car in a hypothetical urban setting. (left, center) Two snapshots, taken just a few seconds apart, show chlorine gas spreading quickly at street level. (right) An overhead perspective, taken 18 minutes postrelease, shows the gas flowing between and over buildings.

training, the code is fast enough for eventual use in NARAC real-time operations.

### Watching Chlorine Gas Disperse

Livermore researchers use Aeolus and other NARAC codes to help strengthen existing local government plans for responding to the release of a toxic chemical such as chlorine. A train transporting liquefied chlorine typically pulls tank cars that individually hold 90 tons of gas. A single ruptured chlorine tank car could cause thousands of casualties from gas inhalation.

In an effort led by Livermore chemist Sarah Chinn, Laboratory chemists and engineers use simulations to understand how buildings affect the dispersion of gas from



SceneWorks-generated visualizations of Aeolus simulations show chlorine gas rises much higher (left) in an urban environment than (right) in an open field. The red and white pole measures 100 meters tall.


An Aeolus-simulated chlorine gas release (red) near downtown Houston, Texas, spreads quickly following a train derailment.

a ruptured chlorine tank car in a downtown urban location. As liquid chlorine pours out from the car, it quickly turns into a toxic cloud carried downwind through city streets. Simulations show that in 5 minutes the gas cloud travels several blocks. However, along the way, it is also trapped inside courtyards, forming "hot zones."

The Aeolus simulations show that although chlorine is a heavy gas, the cloud can be swept upward to the tops of multistory buildings. Within about an hour, most of the toxic cloud is blown downwind and dispersed. However, some of the cloud lingers in high concentrations in alleys and behind buildings. Chinn says that the simulations give emergency planners a more realistic idea of such an incident's consequences, both in terms of immediate and long-term health effects and of cleanup. Team member Maureen Alai explains, "Not every responder would necessarily consider how buildings affect dispersion. Yet a responder could encounter pockets of high concentrations after the cloud appears to have dispersed. Other models that do not resolve individual buildings show the gas remaining closer to the ground." Ultimately, local planners can incorporate this knowledge into their own emergency response planning efforts and tailor the plans to the specifics of their own community.

As part of an OHA project to assess disaster response capabilities, Livermore engineers Robert Greenwalt and Wilthea Hibbard use advanced simulations to investigate the effects of a large toxic chemical release, examine the capabilities of local response systems, and determine best practices to maximize the lives saved. OHA managers asked the researchers to study two locales: Houston, Texas, with one of the biggest concentrations of chemical plants in the world, and an indoor sports and entertainment arena in Boise, Idaho, with virtually no nearby chemical industries.

The scientists are assessing Houston's and Boise's emergency response plans in the context of five separate chemical incidents, including a hypothetical large chlorine gas release from a train derailment. Model simulations and experimental measurements are used to estimate changing chlorine gas concentrations and determine the locations and number of people that would be affected under typical weather patterns. "OHA's focus is on saving lives," explains Greenwalt. "We are examining the entire response system, from initial exposure until the last casualty is released from the hospital. We use the gas plume for estimating the number of people who will be exposed to determine how local emergency rooms will be affected."

## Looking for Planning Gaps

"We are looking for any gaps in a city's emergency response capabilities," says Greenwalt. "Our aim is to suggest improvements." The long-range goal is to produce a generic document showing any city how to evaluate its emergency response system with respect to a chemical release.

The two engineers made several trips to both Houston and Boise, where they met with local emergency responders. At the arena, Greenwalt and Hibbard measured the indoor airflow to determine how quickly the release of a toxic gas would spread through the structure. They also measured how quickly an external plume of gas would flow into the building. Finally, they studied the methods firefighters would use to conduct large-scale decontamination of arena spectators.

Hibbard found that the proper response to a toxic gas release such as chlorine depends on a citizen's location. People in an arena should leave at once if a toxic gas release occurs inside the facility. However, in the case of an outdoor toxic gas release, buildings can provide considerable protection. In this instance, the people should shelter in place, close windows and doors, turn off air-conditioning and heating systems, move to interior rooms, and remain in those rooms until further notice.

Livermore researchers are also developing toxic chemical release scenarios for Georgetown University's Emergency and Disaster Management master's program, a collaboration between the university and Livermore. "The

Photograph courtesy of Brooke Buddemeier

program is designed to prepare students for careers in emergency and disaster management and to become thought leaders in the field," says Livermore's Nancy Suski, deputy program director for academic partnerships, who serves as the disaster management program's executive director. As part of the students' training, they visit Lawrence Livermore to learn how researchers predict the effects of potential hazardous threats. Suski says that scenario-based learning founded on simulations places students in the center of a disaster so that they can "see," for example, how a gas might be blown through a cityscape. Graduates of the program often go on to help cities respond to human-caused and natural disasters.

Livermore modeling expertise is used in other types of potential disaster scenarios including the natural contamination or deliberate poisoning of a city's food supply. Such events could occur, for example, from radioactive fallout settling on fields outside of an urban area or inadvertent contamination of food at a processing plant. The accidental or deliberate contamination of food has been named one of the major global public health threats in the 21st century. Experts contend that strengthening surveillance and response plans constitutes the most efficient and effective way of countering food terrorism.

In an effort to improve response planning for food bioterrorism, Livermore engineer Tom Edmunds and colleagues have investigated potential scenarios involving the deliberate poisoning of a city's food supply. His research uses systems analysis to examine how an attack might be perpetrated, how quickly symptoms would appear, the extent of casualties, and potential mitigation measures. In one scenario, the researchers developed a model that simulates all the steps involved in a milk-poisoning event, including distribution through the supply chain and response to the incident.

With the help of experts from the California Department of Public Health, Edmunds' team developed a human dose response model to estimate when symptoms first appear and hospital emergency personnel begin seeing their first patients. The model also calculates when hospitals would need to order additional doses of antitoxin. One important attribute of the model is that it allows authorities to test the effectiveness of new countermeasures against food bioterrorism.

## Realistic Training Is Key

Livermore researchers are also developing methods to make disaster scenarios and response training more realistic. Steve Kreek, who leads Livermore's Nuclear Detection and Countermeasures Research Program, and colleagues have been working with the Neptune Coalition, a northern California consortium of more than 50 federal, state, and local agencies from the State of California, U.S. Coast Guard, and nine Bay Area counties. The Neptune Coalition is developing a regional response for maritime operations, and local police marine units are deploying pilot-scale radiation detection systems developed at Livermore.

The Neptune Coalition executive board includes Livermore scientists who provide technical advice on exercise planning and concepts of operation. "Thorough plans are essential," says Kreek, "and realistic training of local responders is critical."

Students from Georgetown University's Emergency and Disaster Management master's program learn about special hazardous material operations during a visit to a Livermore–Alameda Country Fire Station located at Lawrence Livermore. (Photo by George A. Kitrinos.)

The Livermore representatives help improve training for responding to a nuclear incident, such as determining the extent of radioactive fallout.

However, training first responders to locate and identify radiation sources is limited by the materials that can be deployed. Actual nuclear materials cannot be deployed for safety, security, and cost reasons. Rather, surrogate radiation sources must be used, but they typically do not represent an actual radiation threat. "At this time," says Kreek, "training is hampered by its artificiality. We want robust training scenarios for a postdetonation radiological or nuclear event, but we can't distribute radioactivity around a city."

A Livermore-designed device called the Spectroscopic Injection Pulser (SIP) aims to create far more realistic training. The device injects a simulated radiation signal (statistically valid energy spectra) into a commercial gamma-ray detector. The signal is injected pulse by pulse, as would be the case using a real radiation source. With SIP, the simulated signals appear the same to the users as a real radiation source. However, because SIP produces a synthetic signal, one can represent far more realistic scenarios such as wide-area contamination and complex compositions that vary with time and location. The prototype device can be attached to the exterior of a detector or later could be integrated into the instrument.

The Livermore team is currently working with a number of detector manufacturers, encouraging them to include the equivalent of a standard interface port (analogous to a USB port) with their next-generation detection equipment to accommodate SIP. The system was recently demonstrated as a "plug and play" with a commercial high-resolution gamma detector commonly used by responders. The team plans to miniaturize the Laboratory prototype as well as expand the capability of the device to simulate electronic signals for detectors used in releases of toxic chemicals and explosives. "The approach lends itself to just about any instrument that makes a physical measurement," says Kreek.

## Sound Science Is Cornerstone

Livermore continues to provide advanced modeling, technical assessments, briefings, and reports to inform federal, state, and local response and recovery planning activities. "Every community is different," says Waters. "Sound science is the cornerstone of good response planning, but it must be tempered with city-unique operational realities and strategies."

Planning for a potential terrorist event is not a pleasant task. However, Livermore researchers are showing that when planning is based on science and advanced modeling, the payoff could be tens of thousands of lives saved.

*—Arnie Heller*

**Key Words**: Aeolus code, chlorine gas, Department of Homeland Security (DHS), Federal Emergency Management Agency (FEMA), improvised nuclear device (IND), National Atmospheric Release Advisory Center (NARAC), Office of Health Affairs (OHA), Spectroscopic Injection Pulser (SIP).

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# Energy Applications DRIVE Carbon Aerogel Innovation

FOR decades, Lawrence Livermore researchers have refined methods for bringing together the best features of two remarkable materials, carbon and aerogels. Aerogels are networks of nanometer-sized particles that are interconnected to create sturdy, low-density, high-surface-area foams. The marriage of carbon and aerogels produces three-dimensional (3D) materials suitable for battery electrodes, catalyst supports, and other applications in the energy realm, thanks to their high surface area, open-pore structure, fine pore size, electrical conductivity, environmental compatibility, and chemical stability.

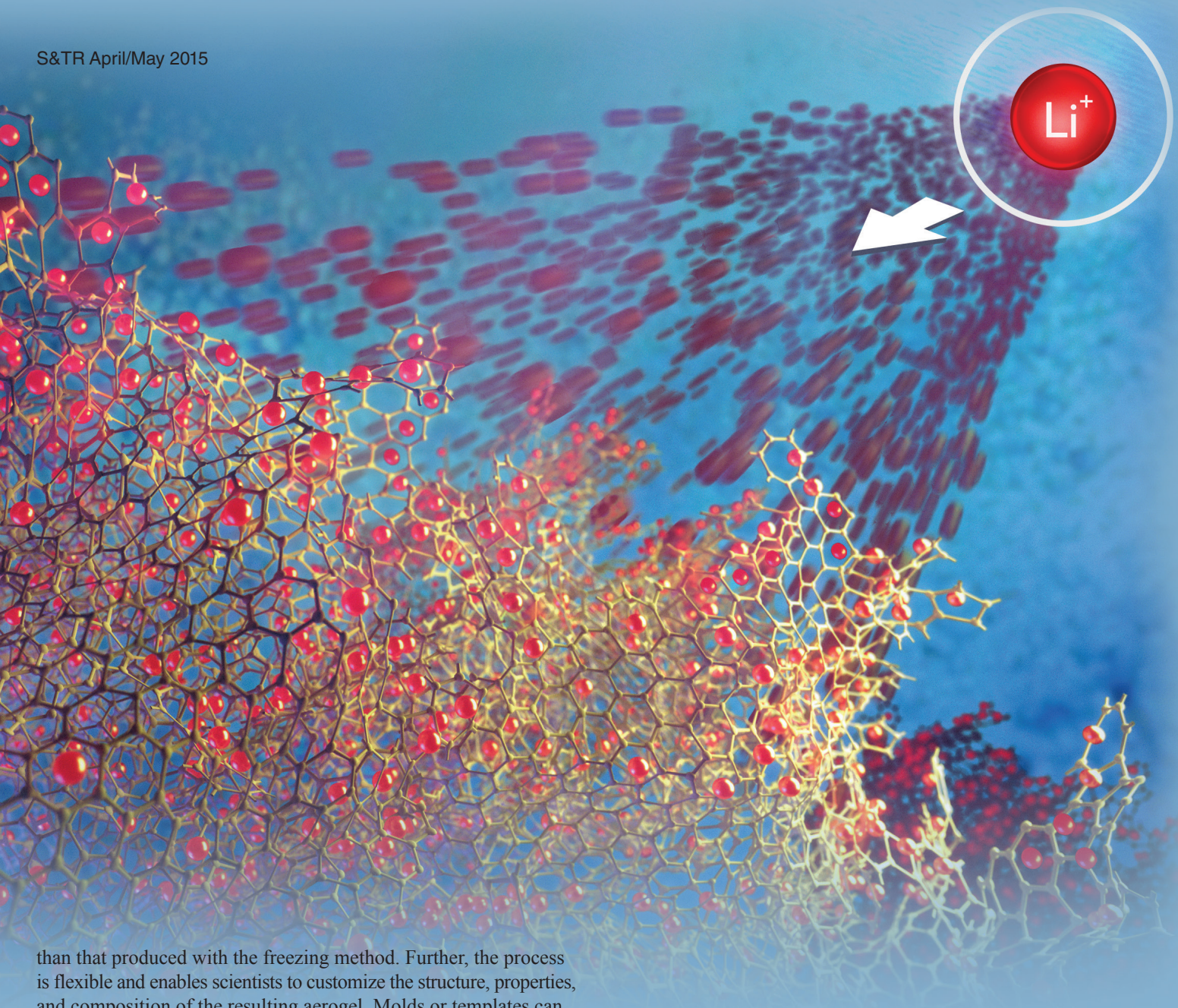
Two recently discovered forms, or allotropes, of carbon offer an opportunity to improve upon these properties. Graphene, a single sheet of carbon atoms, and carbon nanotubes, made of one or more graphene sheets rolled into a tube, have attracted interest in the scientific community because they offer a combination of mechanical robustness, excellent electrical conductivity, and high surface area, outshining other carbon allotropes. However, use of these promising materials has been hindered by difficulties with organizing multiple nanotubes or sheets of graphene into functional 3D structures, while retaining their special properties. Aware of this need, Livermore researchers have demonstrated that their time-tested aerogel synthesis technique can be adapted for use with these newer allotropes. This approach is enabling them to craft superior materials for energy applications.

## It's Nanotubular

When chemical engineer Marcus Worsley joined the Advanced Materials Synthesis (AMS) Group in the Physical and Life Sciences Directorate in 2006, the researchers were striving to create a carbon-based material that could meet the demanding requirements for onboard vehicle hydrogen storage. Group leader Ted Baumann says, "We needed a better carbon structural framework for energy storage applications, both when it came to basic building blocks and to the extended network." Worsley, who became interested in nanotubes in graduate school, suggested using single-walled carbon nanotubes in an aerogel.

"The original method of making nanotube structures involved creating a suspension of nanotubes in water, freezing them, and then removing the ice," says Worsley. "The nanotubes would be held together by physical interactions, but the material would not be very strong." In addition, this method reduced both the surface area and elasticity exhibited by the individual nanotubes. Alternatively, binder materials could be added for structural reinforcement, but most of these materials diminished the electrical or thermal properties of the nanotubes. Worsley's solution was to use sol-gel chemistry to make a conductive aerogel-based "glue" for holding the nanotubes together.

Sol-gel chemistry, a standard method for making aerogels, involves the reactions of chemicals in solution to produce a suspension of nanometer-sized particles, also known as a sol. (See *S&TR*, May 2005, pp. 24–26.) The particles in the sol crosslink to form a 3D solid network called a gel. An aerogel is created when the liquid in the pores of the gel is removed using a special drying process. Because the individual particles in the aerogel network are held together through chemical bonding, the material is stronger




than that produced with the freezing method. Further, the process is flexible and enables scientists to customize the structure, properties, and composition of the resulting aerogel. Molds or templates can be used to imbue the material with specific structural features, and additives can be incorporated to enhance the material's electrical, thermal, or mechanical properties.

When the AMS team introduced a few carbon nanotubes into a standard carbon aerogel solution, they noted that the aerogel particles attached to the walls of the nanotube bundles and successfully bound them together. After gradually changing the proportions through a series of experiments, the team eventually arrived at a mixture that was mostly carbon nanotubes with a sparse population of aerogel particles. This carbon nanotube aerogel was mechanically robust, highly compressible, and more electrically and thermally conductive than carbon nanotube 3D structures created through other methods.

Because of their high surface area, electrical conductivity, and compressibility, the newest members of the carbon aerogel family—carbon nanotube and graphene aerogels—show great promise for energy storage applications such as batteries and capacitors. Shown is an artist's rendering of lithium ion storage on graphene sheets. (Rendering by Ryan Chen.)

## Process Takes Shape

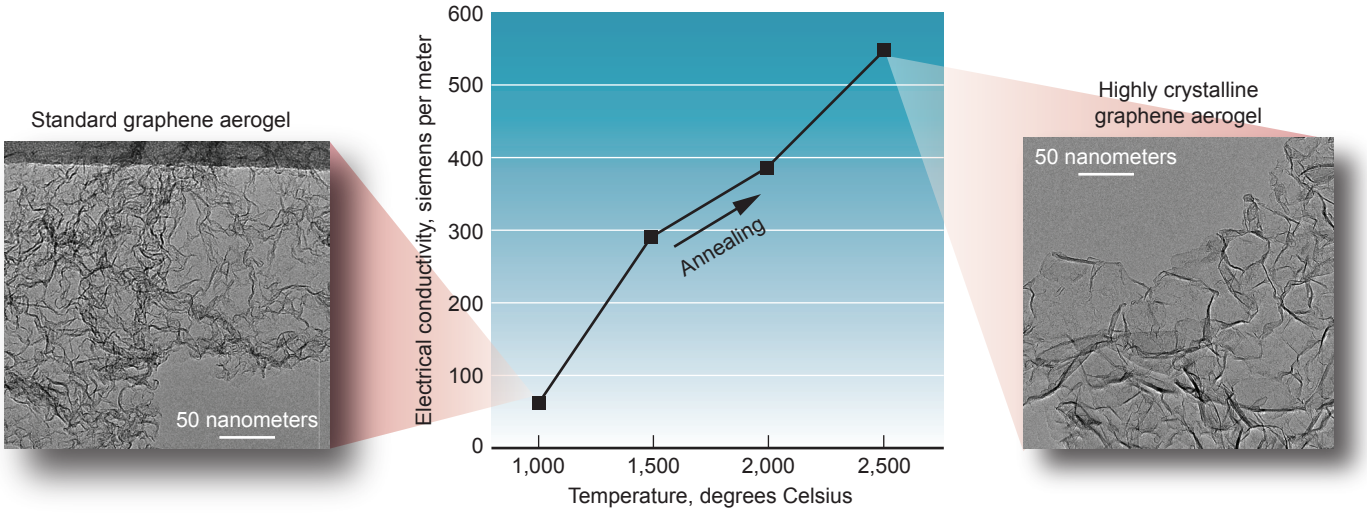
"Over time," explains Baumann, "graphene replaced carbon nanotubes as the material of choice because it has more favorable properties for energy storage, such as higher surface area." Worsley found a creative way to assemble 3D foam structures using graphene building blocks while maintaining many of graphene's desirable properties. Other researchers typically have made 3D graphene structures using the same method they have used to make carbon nanotube assemblies—by suspending graphene oxide nanoparticles in water and then freeze-drying them. This method, however, yields small, low-quality crystal structures with poor physical properties. Worsley and his AMS colleagues used their carbon-nanotube-aerogel synthesis technique to make graphene aerogels bound solely through intermolecular attraction with 100 times better electrical conductivity than 3D graphene structures. The Livermore approach is also more scalable and much less costly than other 3D graphene synthesis methods.

Worsley and University of California (UC) at Berkeley professor Alex Zettl have since led a successful effort to enhance the physical, mechanical, and electrical properties of graphene aerogels. By baking the newly formed graphene aerogel in helium at temperatures between 1,500 and 2,500°C, the scientists produced a material with far fewer structural defects and 10 times larger crystals—up to 150 nanometers in diameter—than previously reported graphene aerogels.

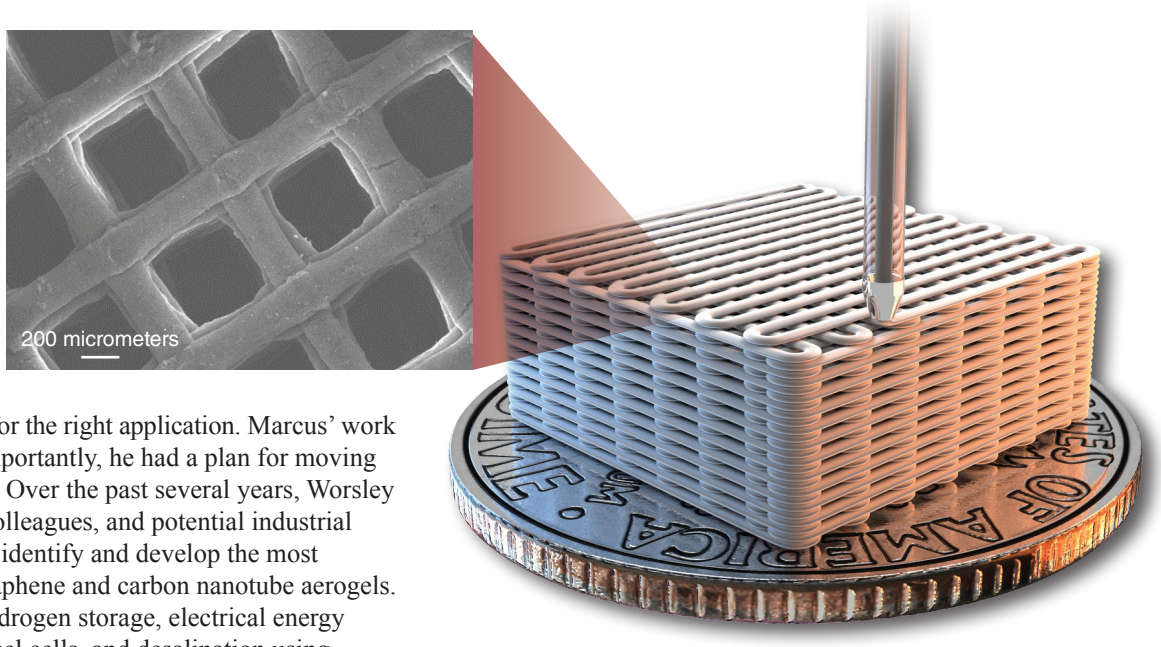
"Graphene has a very specific Raman spectroscopy signature," notes Worsley. "We found that by heating the graphene to about 2000°C, its Raman signature changes. Basically, we are crystallizing the aerogel to the point where it looks like single-sheet graphene." By improving the quality of the individual graphene sheets comprising the aerogel assembly through the extra heating step, the team can produce superior bulk aerogel materials. The new aerogels are not only more stable at higher temperatures but also up to 10 times as conductive and up to 14 times as stiff as other graphene oxide-based aerogels.

## From Test Tube to Patent

The AMS Group's original and technologically relevant carbon-nanotube and graphene-aerogel synthesis work has generated a portfolio of intellectual property that the Laboratory has begun licensing and using to develop partnership and cooperative research agreements with industry. Annemarie Meike, a business development executive in the Laboratory's Industrial Partnerships Office (IPO), has spearheaded the commercialization efforts for these materials. She observes, "Worsley's work results in strong patents because it can serve as a base material for many applications. It is not unusual to see a delay before a new technology's applications and processes emerge. However, because Livermore is known for its aerogels, and the materials have been commercialized in the past, Worsley's work is generating a great deal of interest at an early stage."




Three-dimensional (3D) graphene structures are created using sol-gel chemistry and "baked" to achieve high-quality crystals within the graphene sheets. Their properties approach those of individual graphene sheets isolated through exfoliation, the optimal method for producing graphene.




Three-dimensional printing technology can be used to create graphene aerogels with a highly ordered pore structure and thus more predictable properties. An artist's rendering of a printed 3D aerogel microlattice is shown with (inset) a scanning electron micrograph of the actual structure.

Hannah Farquar, an IPO market research analyst, notes, "After two scientists from the University of Manchester were awarded the 2010 Nobel Prize in Physics for their graphene experiments, many scientists began exploring how to make the promise of graphene a reality, which required the right technology for the right application. Marcus' work was innovative and, just as importantly, he had a plan for moving forward with the technology." Over the past several years, Worsley has worked with IPO, other colleagues, and potential industrial collaborators and licensees to identify and develop the most promising applications for graphene and carbon nanotube aerogels. These applications include hydrogen storage, electrical energy storage, catalytic support in fuel cells, and desalination using capacitive deionization.

While carbon aerogels have been used in all of these research areas before, the new materials offer additional benefits. "The more surface area the aerogel has for a given volume, the more energy it can store," explains Worsley. "Not only does graphene have greater electrical conductivity and energy and power densities for a given mass than other options, but it's also compressible. Because aerogels are very low density, they can occupy a lot of space, but ours can increase in density by eight times without losing performance."

Each application has necessitated some customization of the new materials' structure and properties. For example, both the surface area and the pore structure of traditional carbon aerogels needed to be modified to meet the challenging material requirements for onboard vehicle hydrogen storage. To this end, Livermore researchers, in conjunction with researchers at the California Institute of Technology, have used thermal activation. The controlled burn off of carbon from the aerogel structure in an oxidizing atmosphere creates new micropores (smaller than 2 nanometers) that serve as favorable sites for hydrogen uptake.

In addition, aerogels used in electrodes need very high energy densities for practical applications. Livermore researchers from the AMS and Nanoscale Integration Science and Technology groups teamed up to successfully coat the surface of graphene aerogels with anthraquinone and other molecules that undergo reduction–oxidation reactions. These coatings have yielded up to a three-fold increase in capacity for energy storage devices such as batteries and supercapacitors.

Finally, as supportive structures for catalysts, the surface of an aerogel must be modified with the addition of catalytic nanoparticles. (See *S&TR*, April/May 2009, pp. 23–25.) The AMS Group, in partnership with UC Berkeley professor Roya Maboudian and her research team, has produced hydrogen-sensing, platinum-decorated graphene aerogels with high catalytic efficiency at a reasonable cost.

## Better with Boron

Meanwhile, the AMS Group continues to explore how to build a better aerogel. Currently, the researchers are targeting the pore networks of graphene aerogels, which, until now, have had a fairly random structure. With an engineered structure, realized through 3D printing, these aerogels could achieve even better performance. The researchers have been collaborating with Chris Spadaccini's additive manufacturing team to develop a printable graphene-based ink and modify a 3D printing method called direct-ink writing to

## Livermore's Enduring Contributions to Aerogel Science

Lawrence Livermore researchers have pioneered aerogel chemistry and application for more than 30 years. The lightest known solids, aerogels are also quite strong because of their complex cross-linked internal structure, which gives them among the highest internal surface areas per gram of any material. They also feature outstanding thermal insulating and acoustic properties. Aerogels are readily formed through sol-gel chemistry, in which nanometer-sized particles develop and connect with one another to create a three-dimensional solid network. The flexible sol-gel process has enabled Laboratory researchers to synthesize a broad range of aerogels including silica, carbon, and many metals and oxides.

In the early 1980s, Livermore scientists researching nuclear-pumped x-ray laser systems began experimenting with silica aerogels for laser targets. Over the next decade, these researchers extended aerogel technology by creating superlight silica aerogels, aerogels doped with other materials, and aerogels made of carbon. Ted Baumann, leader for the Advanced Materials Synthesis Group, which creates aerogels for targets and other applications, notes, "For laser physics experiments, aerogels are interesting because of their tunable density, which allows us to make changes easily, and submicron features, which help to reduce hydrodynamic instabilities. Carbon aerogels are also low-*Z* materials, which is an important advantage both for experiment design and data collection."

Livermore scientists quickly recognized that carbon aerogels were also useful electrode materials and ever since have been exploring their utility in supercapacitors and rechargeable batteries, thermal insulation, adsorbents, and advanced catalyst supports. Another notable application for carbon aerogels has been water purification. Researchers have developed novel approaches for removing contaminants such as uranium and arsenic from groundwater and salt from seawater (See *S&TR*, January/February 2013, pp. 16–19.)

Because the sol-gel process confers control over composition and structure on the nanometer scale, aerogels have also been key to making energetic materials—substances that store energy chemically—with improved or entirely new properties. By mixing an oxidizer and a fuel at the nanometer scale, Livermore researchers have created energetic composite materials with more uniform structure and better performance. (See *S&TR*, October 1999, pp. 19–21.) Further, these materials are easier and safer to synthesize than energetic materials made with traditional methods.

Laboratory scientists are still finding new applications for "old" aerogels. During the Stardust project, for instance, silica aerogel was used to collect and return samples of fast-moving cosmic dust from space. Study of the particles shed light on the solar system's formation. (See *S&TR*, April 2007, pp. 5–11.)

Laser physics experiments such as high-energy-density science, ignition, and plasma physics, the original impetus for aerogel research at the Laboratory, continue to help propel aerogel innovation. Today, many targets fielded at the Laboratory's National Ignition Facility, the world's most energetic laser, incorporate aerogels. (See *S&TR*, September 2006, pp. 23–25.) "The aerogel requirements for laser experiment targets are constantly evolving and becoming more demanding with each iteration of experiments," says Baumann. "For instance, the experimental designers are now requesting aerogel materials that possess extreme and precise density gradients. Designing aerogels to meet these requests is an ongoing challenge."

accommodate aerogel processing. Preliminary results are promising. The 3D-printed graphene aerogels produced thus far with this method are lightweight, highly conductive, and extremely compressible. In addition, their structural integrity can be maintained over multiple compression cycles.

Zettl's team, in conjunction with AMS researchers, has created the first boron nitride aerogels using high-quality graphene aerogels as a template. Boron nitride is typically a two-dimensional material with a similar structure to graphene. Its high thermal conductivity and thermal stability make it attractive for sensor applications. Worsley says, "For the first time, we were able to convert the graphene completely to boron with no leftover carbon, because the low porosity and high surface area of our graphene aerogels creates very little bulk material and enables more efficient conversion."

Carbon nanotube, graphene, 3D-printed graphene, and boron nitride aerogels mark the latest in a long line of remarkable aerogel accomplishments (see the box above) motivated by the institution's and the nation's security, energy, and scientific needs and made possible by the AMS Group's aerogel architects. Baumann says, "It is very satisfying to see the materials we create put to use."

*—Rose Hansen*

**Key Words:** aerogel, allotrope, battery, boron, carbon, catalyst, desalination, direct-ink writing, energetic material, graphene, laser target, micropore, nanotube, sensor, silica, sol-gel chemistry, Stardust project, supercapacitor, surface area, three-dimensional (3D) printing.

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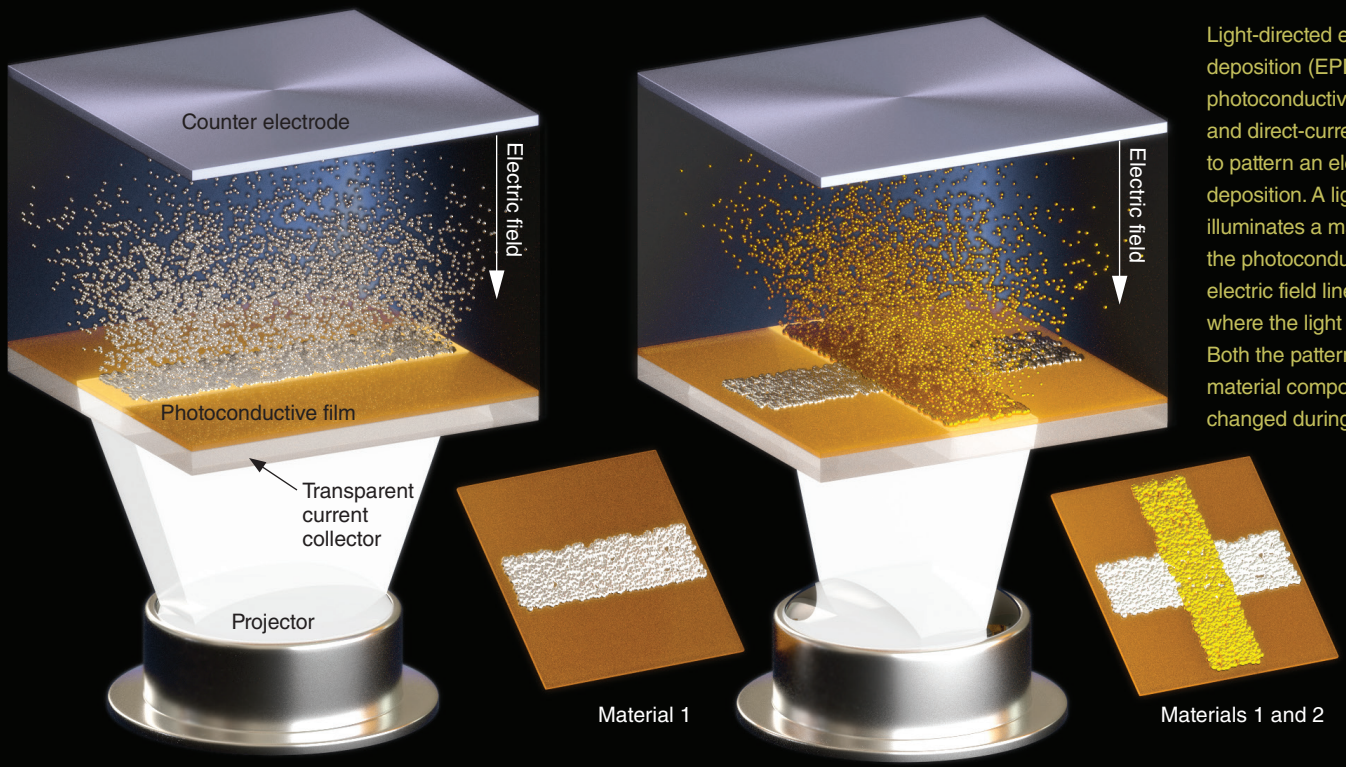
# A Guiding LIGHT for Designer Materials

THE ability to fabricate three-dimensional (3D) parts and other components with the utmost precision has always been a necessity for Livermore. Time and painstaking effort are dedicated to producing objects needed for many of the Laboratory's missions, including stockpile stewardship. Additive manufacturing (AM) processes have recently shown promise for improving the quality and repeatability of components and for significantly reducing the time and cost associated with their production. (See *S&TR*, January/February, pp. 4–11.) In addition, AM may also enable the development of novel materials with unique properties. (See *S&TR*, March 2012, pp. 14–20.)

Several AM approaches are under development at Livermore. Electrophoretic deposition (EPD) uses an electric field to drive suspended colloids from a solution onto a conductive substrate. Originally developed for applying corrosion-resistant paint to car bodies, EPD has evolved into a process that allows a wide range of materials to be deposited on various surfaces, including ceramics, metals, polymers, living cells, and biological material. However, the process is limited because a material can only be deposited uniformly across a surface, and the pattern cannot be changed as the material is built up.

As part of a study funded by the Laboratory Directed Research and Development Program, Livermore scientists are transforming EPD from a simple coating process to a new AM capability for freely creating 3D structures. "We have demonstrated multimaterial patterning using a light-directed EPD technique that enables two or more materials to be placed next to and on top of each other," says Livermore materials scientist Andrew Pascall. "Our work has shown that 3D composite structures are possible." A team led by Pascall, which includes materials scientist Joshua Kuntz and computational engineer Luis Zepeda-Ruiz, is also developing improved simulation and modeling capabilities to




Light-directed electrophoretic deposition (EPD) uses photoconductive electrodes and direct-current electric fields to pattern an electrode during deposition. A light source illuminates a mask pattern onto the photoconductive film. The electric field lines concentrate where the light hits the film. Both the pattern and the material composition can be changed during deposition.

better understand the deposition process. The models will help visualize the fundamental physics of deposition that control whether colloids deposit randomly on a surface or whether they form dense crystal structures.

With light-directed EPD, researchers can use a much larger breadth of materials as compared with other AM tools, because the technique relies on particle size and surface charge rather than on the actual chemistry of the deposited material. In addition, EPD techniques offer submicrometer lateral precision and the potential for large-scale production. Kuntz explains, "With light-directed EPD, our goal is to fabricate functional and graded 3D composites for a wide range of Laboratory and industrial applications."

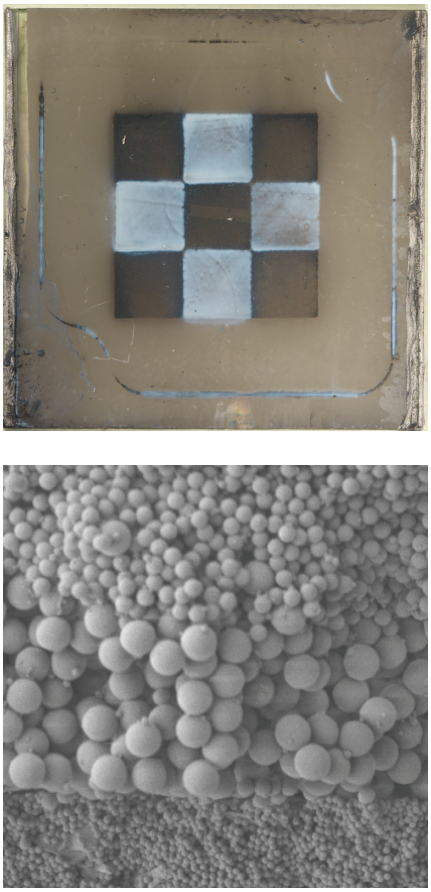
## Drawn to the Light

In traditional EPD, a liquid suspension containing electrically charged micro- to nanoscale colloidal particles is flowed into a deposition cell with opposing electrodes. When an electric field is applied to the deposition cell, the surface charge of the particles causes them to flow parallel to the field lines until they hit and stick to the electrode's surface. A drawback of traditional EPD is that the electrodes are static contacts, and therefore they are not changeable during deposition. As a result, gradients in the deposit composition can be made only in a direction normal to the electrode surface. Static contacts also restrict the dimensionality of the deposited structure. "Movable counter electrodes have been investigated as a method for depositing materials in targeted areas, but these approaches have not demonstrated multimaterial patterning and are difficult to scale," says Pascall. "A dynamic, reconfigurable electrode is needed for patterning in all directions."

The Livermore team's light-directed EPD technique uses photoconductive electrodes and direct-current electric fields to pattern the electrode during deposition. In this scheme, a photoconductive film is grown on a transparent conductive layer, yielding a light-responsive electrode. The electrode's conductivity increases where the light hits the film, causing the electric field to concentrate at that location. During deposition, the illumination pattern on the photoconductive electrode can be changed dynamically. Material composition and gradients can also be adjusted.

Altering material composition or particle size requires the ability to change material in the deposition cell. The team's flow-control system allows one material to be flowed into the cell in a particular pattern, then flowed out, and a new material to be injected as the pattern is changed. Without such flow control—which most other EPD techniques lack—the composition cannot be changed as one changes the thickness away from the substrate. Thus, light-directed EPD can rapidly pattern multiple, diverse materials to produce 3D composites to exacting specifications.

Another benefit to light-directed EPD is that void space can be incorporated into a composite structure by depositing a material within a layer that can be subsequently removed with postprocessing. "Typically, EPD provides a structural 'green body,' similar to a sandcastle or an unfired ceramic," says Kuntz. "After the object is fabricated, chemical curing or some other thermal process is needed to induce physical bonding throughout the structure." The ability to add in and then burn out excess materials gives light-directed EPD an edge in producing 3D composite structures, and it is the only EPD technique with the demonstrated capability to produce such structures over large areas and with fine resolution.



Livermore researchers use light-directed EPD to produce composite materials by precisely placing two or more materials in the plane of the electrode. (top) In this case, a metal (black) and ceramic (white) composite has been formed. (bottom) Layered composite materials can also be formed via traditional EPD, such as in the case of these different-sized polymer spheres. The largest spheres shown here are 1 micrometer in diameter. Arbitrary three-dimensional composites can be produced by combining these two modes.

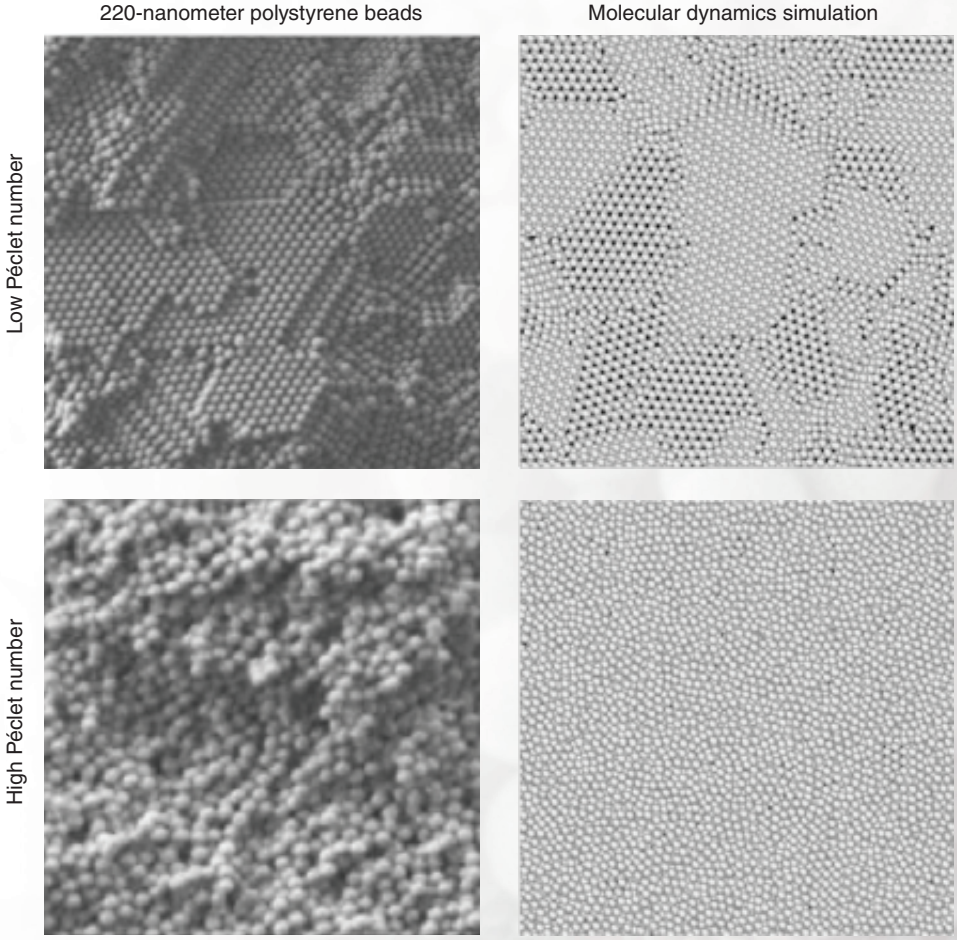
## A Predictable Arrangement

Computational modeling has become a powerful tool for helping researchers study complex physics processes. For this

reason, the light-directed EPD research team is turning to advanced simulation to predict the fundamental physics of deposition, which in turn could speed development of improved colloid suspensions. "We are applying direct element modeling techniques to simulate individual nanoscale particles—ten to hundreds of nanometers in size—in colloid suspensions," says Zepeda-Ruiz. "These models help us to understand the deposit morphology. We want to know what process parameters lead to ordered versus amorphous deposits."

Simulations are designed to describe how the colloidal particles move in the electric field and how they interact with each other and the substrate surface. "An EPD model is a mesoscopic particle simulation that incorporates the essential electrokinetic and hydrodynamic forces and the particle–particle and particle–electrode interactions that are especially relevant in the assembly of colloidal particles in 3D crystalline lattices," says Pascall. "From the models, we can see how single or multiple colloids will adhere to a particular surface as well as the difference between the deposition rates and self-diffusion abilities of the particles."

The team theorizes that the particles' degree of ordering is controlled by the Péclet number—a variable, directly proportional to the electric field, that compares how fast colloids arrive at the electrode surface versus how fast they diffuse laterally across it. By modeling particle deposition as a function of the Péclet number, the team can see exactly how the particles are arranged on the electrode and whether they form crystalline arrays or deposit randomly. "We are modeling a combination of experimental parameters, different materials, solvents, and particle sizes," says Zepeda-Ruiz. "We've shown that a low Péclet number or low electric field results in an ordered deposit and that the other extreme is also possible. With a high electric field or high Péclet number, the result is a highly disordered deposit."




A comparison between experiments using polystyrene beads and molecular dynamics simulations shows the effect of electric field (high or low Péclet number) on the microstructure of the deposited material. The Péclet number can be used to control microstructure over a range of particle sizes.

The team has run experiments using polystyrene particles deposited over a range of Péclet numbers to validate the computational efforts. "The models allow us to describe the ordering more precisely, which helps us interpret experiments and predict behavior," says Zepeda-Ruiz. "With properly validated models, we can decrease the time needed to develop productive, focused experiments. Variables are much easier to change independently in a simulation than they are in an experiment, so the models can save time by helping us achieve a desired result more quickly."

Using computational techniques to model large-scale electrophoretic deposits at the micro- to nanoscale are vital to transforming light-directed EPD into an AM technology. "We're not running these simulations simply for knowledge's sake but rather to better understand the method itself and the performance of materials for a variety of applications," says Kuntz. At a larger scale, the group is evaluating how dynamic light patterns alter the electric field lines and colloid trajectories in a deposition chamber. Such information will allow them to control patterning during deposition for improved 3D structural fidelity.

## Just the Beginning

George Brewer, the man who is credited with developing EPD for Ford Motor Company in the late 1950s, once said that 150 person-years of research elapsed between the initial EPD concept being devised and the first EPD-coated car rolling off a production line. Transitioning EPD to a fully automated AM technology will also take time, but the adjustments Livermore has made to this technique are already yielding beneficial results. Flow-controlled EPD, for example, is currently being used to create new composite energetic materials and composite armor for defense applications.

In the future, the team envisions light-directed EPD being a completely automated process for AM applications. "This work represents a large step in advancing EPD as a method for fabricating complex, 3D patterned composites," says Pascall. Once fully developed, light-directed EPD may serve as a tool for experiments at the Joint Actinide Shock Physics Experimental Research (JASPER) facility. (See *S&TR*, April/May 2013, pp. 20–23.) Kuntz says, "We're investigating how light-directed EPD could be used to build graded-density impactors—multilayered projectiles made of various graded materials that allow researchers to carefully construct the pressure profile of JASPER experiments."

One day, commercial 3D printers could be based on light-directed EPD, but for now, the team's focus is on demonstrating the technique's versatility and functionality. This process will take time and effort, but the realization of light-directed EPD as a full-scale production capability is well worth the wait. AM technologies such as this represent the next generation of tools for manufacturing and fabrication—tools that will revolutionize American manufacturing and help develop materials with customizable properties for stockpile stewardship and an ever-expanding range of other important applications.

*—Caryn Meissner*

**Key Words:** additive manufacturing (AM), composite material, electrode, Joint Actinide Shock Physics Experimental Research (JASPER) Facility, light-directed electrophoretic deposition (EPD), Péclet number, stockpile stewardship.

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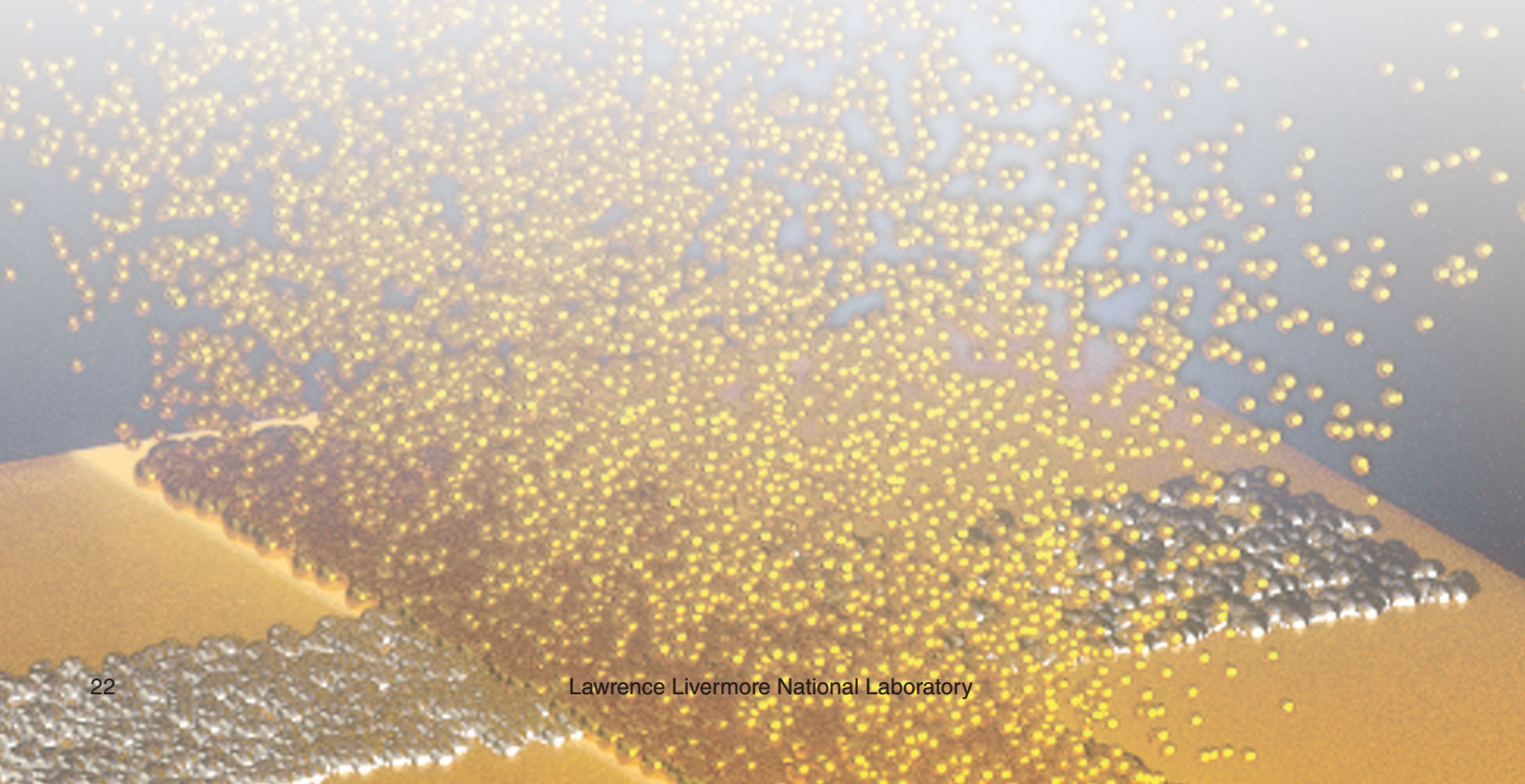
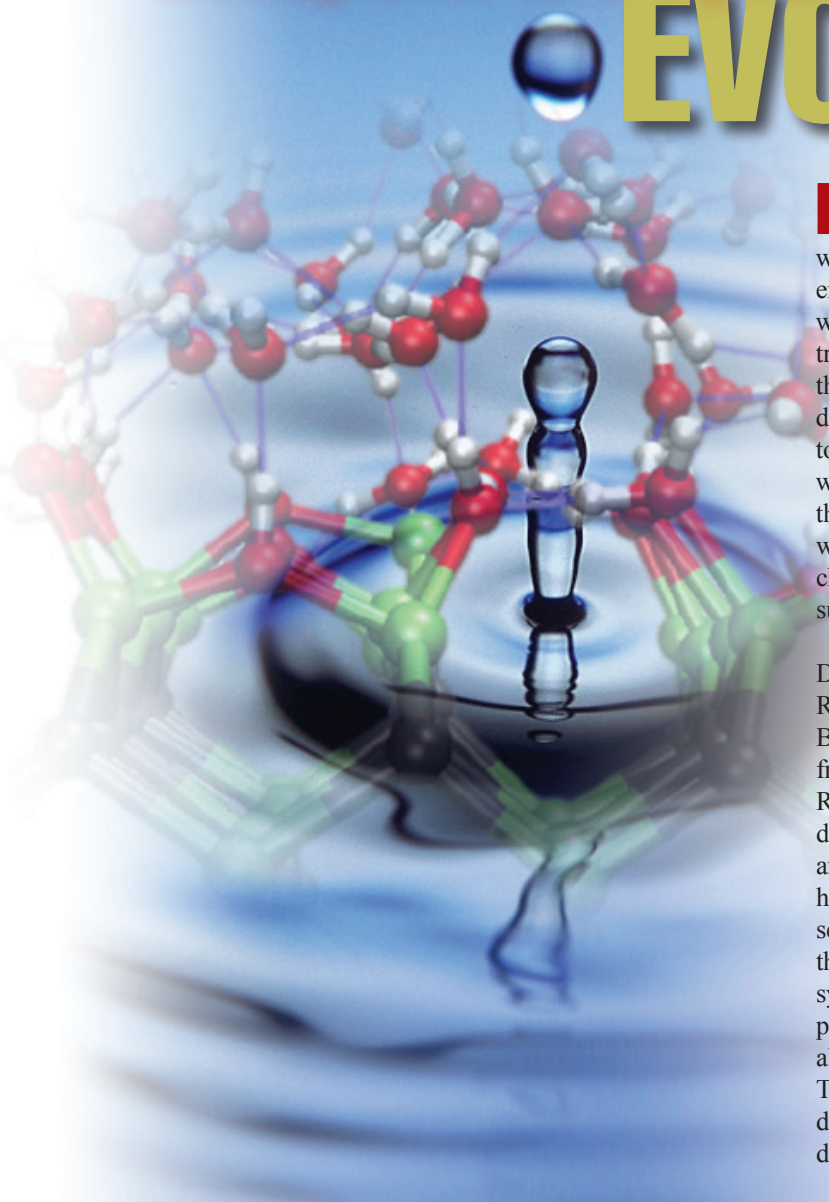


# Diving into the Dynamics of EVOLVING Hydrogen

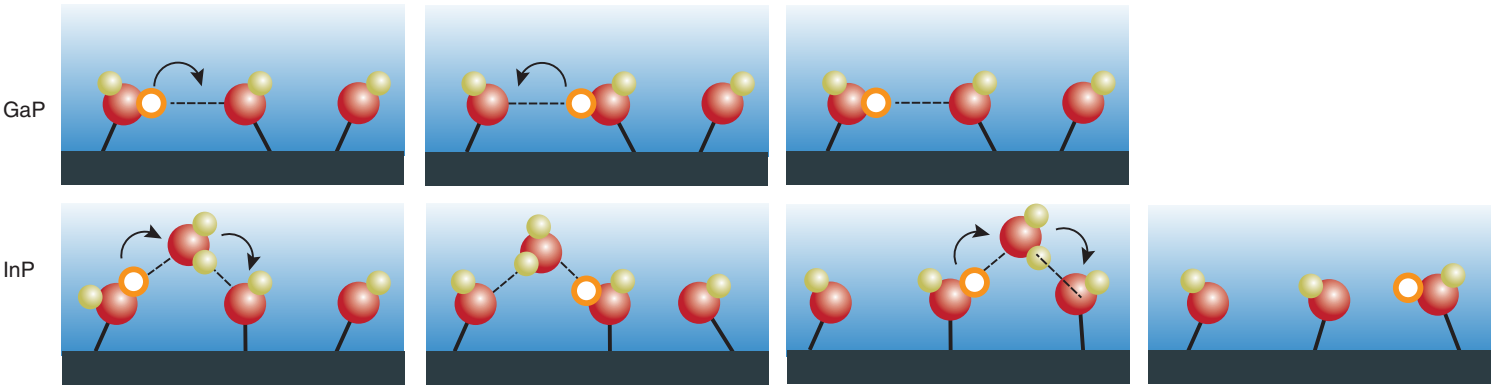


HYDROGEN is the most abundant element in the universe and a basic component of water, along with oxygen. An easy, efficient way to split water into hydrogen and oxygen gas with minimum environmental impact could provide our energy-intensive world with abundant fuel for generating electricity and even powering transportation systems. Livermore scientists are studying a process that uses sunlight—another freely available commodity—as the driver for producing hydrogen fuel. In this scheme, sunlight is used to split a hydrogen atom from a molecule of water at the interface with a light-absorbing semiconductor material. The hydrogen atom then combines with another to form diatomic hydrogen gas ($H_2$), which can be harvested as fuel. It sounds simple, but the specific chemical mechanisms that make this process possible are surprisingly complex and not well understood.

Supported by the Fuel Cell Technologies Office of the Department of Energy's (DOE's) Office of Energy Efficiency and Renewable Energy (EERE), Livermore scientists Tadashi Ogitsu, Brandon Wood, and Wooni Choi are working with collaborators from the University of Nevada at Las Vegas (UNLV) and the National Renewable Energy Laboratory (NREL) in Colorado to investigate the detailed workings of hydrogen evolution reactions. Ogitsu, Wood, and Choi have developed ab initio simulations to model how hydrogen atoms and ions evolve and react in solution and on various semiconductor surfaces at the atomic level. Through their analysis of the chemistry, structure, and dynamics of this complex, interactive system, the researchers are uncovering the nature of fundamental processes that can contribute to efficient hydrogen evolution, as alternatives to those leading to surface corrosion and degradation. The strategies they are devising with this knowledge are key to the development of durable and cost-effective photoelectrochemical devices that can provide cost-effective, clean energy for the future.

## From Water to Hydrogen Gas

One of the goals of EERE is to develop efficient and environmentally responsible solar-to-chemical energy conversion. "It is well established that multiple steps are needed to create hydrogen gas from individual hydrogen ions in solution," explains Ogitsu. (See the box on p. 26.) "Hydrogen atoms adsorbed on the surface of an electrode material play an important role as a reaction intermediate. Hence, we want to obtain a clear understanding of hydrogen adsorption at the atomic level and how this reaction differs from material to material."




(top) Although hopping of adsorbed atomic hydrogen between neighboring surface sites occurs on both gallium-phosphide (GaP) and indium-phosphide (InP), Livermore simulations show that hopping tends to stay more local on GaP because hydrogen forms more rigid bonds with the material. (bottom) InP bonds are looser, allowing the hydrogen to cover more territory in the same amount of time. As a result, InP bonds are more efficient for producing diatomic hydrogen gas, as InP enables individual hydrogen atoms to find more favorable surface sites to interact with other hydrogen species.

EERE funded the team to study the interface between water and various semiconductor surfaces, taking a close look at the chemistry and dynamics of adsorbed hydrogen on various semiconductor surfaces. In particular, the team studied indium phosphide (InP) and gallium phosphide (GaP)—two materials that are strong contenders in the search to create hydrogen fuel by photoelectrochemical water splitting. "Solar water-splitting is hard to do efficiently," notes Wood. "Most systems now being used have a solar-to-hydrogen conversion efficiency less than a few percent. An experimental architecture developed by NREL that incorporates both gallium and indium ($GaInP_2$) has demonstrated a conversion efficiency of about 12 percent. We are looking for ways to pull more energy from this process and make it last much longer."

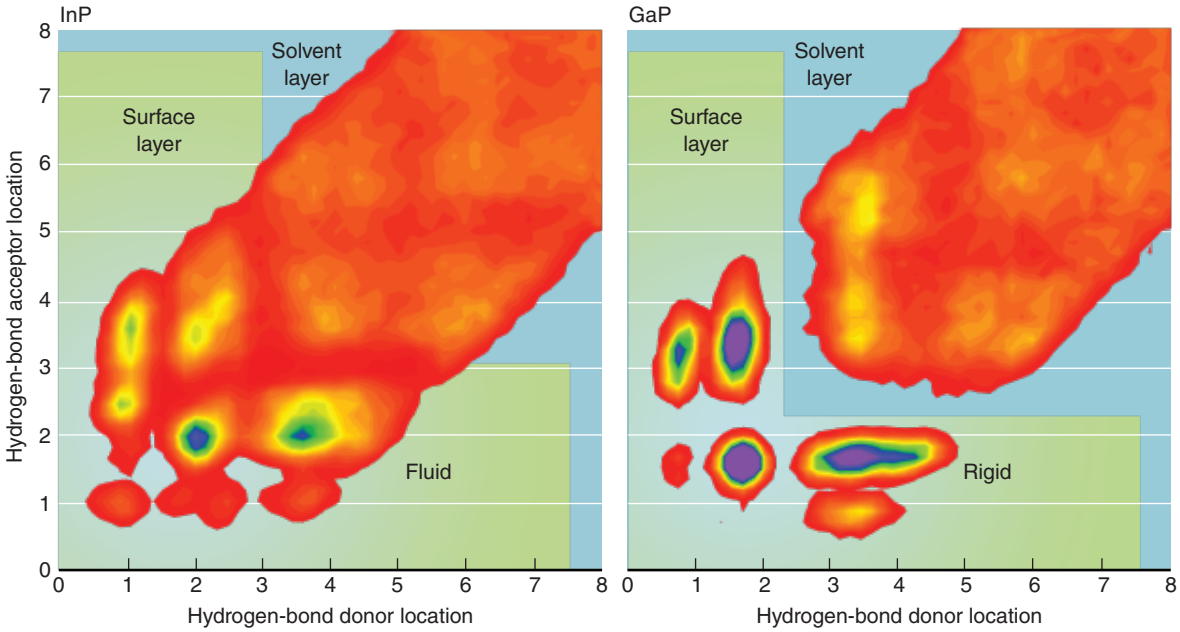
Researchers at NREL have been exploring InP, $GaInP_2$, and other advanced solar-cell materials for their acceptability as solar water-splitting materials. One of the challenges researchers have encountered is pinpointing what governs the efficiency of the hydrogen evolution reaction and thus the conversion of water and sunlight into hydrogen fuel. Another challenge concerns the durability of the semiconductors in an aqueous environment that is often harshly acidic. As a general rule, the most efficient materials also corrode the most quickly, often degrading after only a few hours of operation to the point where they are no longer functional.

"To really understand what is happening, we must consider all the complex chemical reactions and how the various elements interrelate over time," says Wood. "This process had not yet been addressed computationally in any detail, so we looked at the atomic-level interactions between the surface of the solar catalyst–semiconductor materials and the water solution close to the surface." The team needed to model all parts of the system: the atoms forming the semiconductor surface, including nearby water molecules, and the presence of ions and gas molecules at the semiconductor–water interface. The simulation also needed to incorporate effects of the system's ever-changing dynamics and kinetics as the semiconductor interacted with the photons from the Sun and the oxygen from the environment, the constituents from the split water, and the other semiconductor atoms on the surface.

## The Devil Is in the Details

The team turned to molecular dynamics simulations based on first principles to better understand the hydrogen evolution process. The complex, computationally intensive simulations were run on the Laboratory's Sierra and Vulcan supercomputers using a combination of open-source and Livermore-developed codes. What the team discovered was an intriguing link between atomic interface kinetics and the performance and durability of different solar catalyst materials. Ogitsu explains, "Our simulations showed a strong correlation between how mobile the adsorbed hydrogen atom is on a given surface and the efficiency of the system. The importance of mobility suggests that the initial adsorption of hydrogen atoms and the subsequent evolution and release of hydrogen gas molecules occur at physically separated locations. The diffusion between these locations plays a key role in reaction efficiency."

In the simulations, a hydrogen ion extracted from solution does not always simply stick to a single site on the electron-donating semiconductor surface, as is often thought to be the case. Rather, the ion can move freely, or hop, between available sites because of a permanent, thin layer of surface oxygen and hydroxyl, which




Simulations indicate the density of hydrogen bonds formed at the interface between (left) water and InP, and (right) water and GaP, based on the distances of the bond-donor and bond-acceptor species from the material surface. Purple is the region of highest density. Blue and green outline the surface-adsorbing layer and the first layer of solution, respectively. The hydrogen bonds are less structured and exhibit more topological variety for the InP–water interface, which consequently is more fluid and dynamic than the GaP–water interface.

forms a network of bonds that connects neighboring surface sites. Furthermore, the adsorbed hydrogen hops more easily depending on the material. According to the simulation results, the hydrogen is far more mobile on InP than on GaP. Ogitsu says, "This result was unexpected, given that the two materials are similar in their electronic and structural properties."

The reason for the difference lies in the nature of the bonds formed between the adsorbed hydrogen and the molecules and atoms on the surfaces of the two materials. Wood explains, "According to the results of the simulations, hydrogen binds more tightly and rigidly to gallium-phosphide than to indium-phosphide. You could think of gallium-phosphide as having a 'stickier' surface, such as fly-paper." On GaP, the hydrogen makes short hops but is more circumscribed. On the other hand, an adsorbed hydrogen on InP appears to move much greater distances in the same amount of time, and is not confined to one region of the surface. "It's similar to taking a local bus versus an express one," says Wood. "Although you board and disembark at the same locations, the express travels much faster and makes fewer stops in between. Similarly, at the atomic level, InP molecules form looser bonds with hydrogen, facilitating their movement and allowing them to react more readily. As a result, the hydrogen has increased opportunities to find those surface regions that are particularly conducive to reactions with other hydrogen atoms to form $H_2$, thus increasing the efficiency of the system."

In another interesting result, the simulations indicate that the rate at which hydrogen diffuses also depends on the ease with which the adsorbed hydrogen moves into and through the aqueous solution a few atomic layers above the semiconductor's surface. The stiffer, structured bonds at the GaP surface appear to make the water solution close to the surface more icelike and rigid. However, hydrogen mobility relies on molecular exchanges that occur faster and more frequently in the liquid–water system. As a result, the looser, lower-energy bonds between the hydrogen and InP allow the hydrogen atoms to make use of the much faster solvent rearrangements within the near-surface water layer. "In our mass-transportation analogy," says Wood, "the hydrogen ions on the gallium-phosphide bus are constrained to the slow city streets of the surface, whereas those on the indium-phosphide bus can also choose to zip along on the faster, near-surface interstate freeway."

Furthermore, the modeling results suggest that the differences in hydrogen mobility on various materials may also affect a material's susceptibility to corrosion. "Why some materials corrode more readily than others, even when they have similar properties, is still a mystery," says Wood. Some studies indicate that corrosion may occur more easily on surface areas that build up an unwanted local abundance of charge, which suggests a surface that facilitates hydrogen movement would have a natural mechanism for redistributing or neutralizing the accumulated charge, making corrosion less likely. "Our results tend to support the theory that materials with higher hydrogen mobility may be able to 'heal' themselves," says Wood.

## Reality Checks and Rewards

Experimental data serve as a so-called reality check for researchers, who use the data to help validate their theories. The collaboration of Livermore, UNLV, and NREL allows theorists and experimentalists to work together to overcome the challenges associated with hydrogen evolution and accelerate research and development. NREL leads the synthesis effort on improving the durability of carefully tailored compound semiconductors based

## A Formula for Hydrogen Fuel

More than one way exists to create usable energy from the Sun. Photoelectrochemistry begins with an electrochemical system that generates electrical energy from chemical reactions. In the photoelectrochemical process, photons from sunlight provide the initial energy needed to kick-start chemical reactions such as oxidation (in which electrons are released from a molecule) or reduction (in which free electrons attach to a molecule). Photosynthesis—the process used by plants to convert sunlight, water, and carbon dioxide into carbohydrates and oxygen—is an example of a photoelectrochemical process.

Photoelectrochemical water-splitting produces hydrogen gas from water using sunlight and specialized photoactive semiconductor materials, and it holds great promise for converting solar radiation into a storable, nonpolluting fuel. With this technique, the semiconductor surface is immersed in water, and light energy is used to split the water molecules into hydrogen and oxygen in a complex, two-step process. When photons from sunlight hit the semiconductor, if the photons' energies are above a certain level (called the band gap), the system will absorb the energy from the photons. This extra energy allows electrons to move out of their orbits to a higher orbit or excited state where they can travel more freely through the semiconductor material. In a photovoltaic solar cell, these mobile charges are used to directly drive an electronic circuit. In photoelectrochemical water splitting, the energetic electrons are used in a chemical reduction process that transforms hydrogen ions into neutral hydrogen atoms, typically with the aid of a catalyst. The electrons initially accumulate at the surface of the semiconductor, attracting positively charged hydrogen ions that are split off from water. Some of these electrons and ions then combine to form neutral hydrogen atoms that are adsorbed on the surface.

At this point in the hydrogen evolution process, two possible reaction pathways are possible that lead to the formation of hydrogen gas. In one pathway, a neutral, adsorbed hydrogen atom combines with a free hydrogen ion in the water and a second electron to form a molecule of hydrogen gas. This reaction can occur fully on the catalyst, or, as the Livermore team discovered, with the assistance of the semiconductor surface. In the second pathway, two adsorbed hydrogen ions collide and stick together. In both cases, the adsorbed hydrogen atoms on the surface play a critical role in the formation of the final product. Additionally, the team's results indicate that because a significant amount of hydrogen gas is formed on the semiconductor surface via hydrogen surface diffusion, gas production efficiency could be enhanced through this process while using less catalyst material. Understanding the dynamics of these pathways and how the hydrogen ions and adsorbed hydrogen atoms interact with different semiconductor surfaces and in solution is vital to the economic creation and harvesting of hydrogen fuel.

on input from the other team members. UNLV heads experimental characterization of the NREL-provided samples, generating high-fidelity x-ray spectroscopic data from its in situ characterization of different water–electrode interfaces. The semiconductor samples are analyzed at Lawrence Berkeley National Laboratory's Advanced Light Source using x-ray synchrotron spectroscopy, which offers information about the local surface and interface structure. The spectroscopic data is directly compared to simulated spectra based on model surfaces and interfaces provided by the Livermore team, assisted by Lawrence Berkeley scientist David Prendergast as part of a Molecular Foundry project. Through this feedback cycle, the key underlying mechanisms of durability improvement are explored and identified.

Ogitsu, Wood, and Choi's efforts were rewarded last year when their team was named a recipient of DOE's 2014 Hydrogen Production R&D Award, presented by EERE's Fuel Cell Technologies Office (FCTO) in recognition of FCTO-funded R&D in hydrogen production. Their groundbreaking work, which integrates advanced tools and methods in materials theory, synthesis, and characterization, is important for many areas of research, including chemical sensor development, energy storage, and energy conversion. The achievements also exemplify core tenets of the White House's Materials Genome Initiative.

Few interactions are as fundamental as water interacting with a surface, and now researchers have a virtual window into observing these interactions at the very smallest scales. If the results on hydrogen evolution thus far are any indication, atomic-scale observations of such complex processes are bound to yield some compelling and far-reaching insights, proving the old saying that it's sometimes the little things that matter most.

*—Ann Parker*

**Key Words:** ab initio simulation, corrosion, gallium-phosphide (GaP), hydrogen fuel, hydrogen mobility, hydrogen production, indium-phosphide (InP), molecular dynamics, semiconductor, solar-to-hydrogen fuel conversion, water splitting.

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# Patents and Awards

*In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory. For the full text of a patent, enter the seven-digit number in the search box at the U.S. Patent and Trademark Office's website (http://www.uspto.gov).*

## Patents

**System and Method for Compressive Scanning Electron Microscopy**
**Bryan W. Reed**
U.S. Patent 8,933,401 B1
January 13, 2015

**Signal Digitizing System and Method Based on Amplitude-to-Time Optical Mapping**
**Jason Chou**
U.S. Patent 8,934,058 B2
January 13, 2015

**Laser Beam Centering and Pointing System**
**Michael C. Rushford**
U.S. Patent 8,934,097 B2
January 13, 2015

**High Flux, Narrow Bandwidth Compton Light Sources Via Extended Laser-Electron Interactions**
**Christopher P. Barty**
U.S. Patent 8,934,608 B2
January 13, 2015

**Membranes with Functionalized Carbon Nanotube Pores for Selective Transport**
**Olgica Bakajin, Aleksandr Noy, Francesco Fornasiero, Hyung Gyu Park, Jason K. Holt, Sangil Kim**
U.S. Patent 8,940,173 B2
January 27, 2015

**Polymer-Encapsulated Carbon Capture Liquids that Tolerate Precipitation of Solids for Increased Capacity**
**Roger D. Aines, William L. Bourcier, Christopher M. Spadaccini, Joshuah K. Stolaroff**
U.S. Patent 8,945,279 B2
February 3, 2015

**Methods for Isolation and Viability Assessment of Biological Organisms**
**Sonia E. Letant, Sarah E. Baker, Tiziana Bond, Allan Shih-Ping Chang**
U.S. Patent 8,947,657 B2
February 3, 2015

**Super Capacitors with Fibers**
**Joseph C. Farmer, James Kaschmitter**
U.S. Patent 8,958,198 B2
February 17, 2015

## Awards

**Claire Max**, a longtime astrophysicist at Livermore and a faculty member at the University of California at Santa Cruz (UCSC), has earned the **Joseph Weber Award for Astronomical Instrumentation** from the **American Astronomical Society** for her work in adaptive optics (AO). The award is bestowed to an individual for the design, invention, or significant improvement of instrumentation leading to advances in astronomy.

Max received the award for coinventing sodium laser guide star adaptive optics and for shepherding AO from its roots in classified space surveillance to a prominent, essential technology on large telescopes. Her leadership has made near-diffraction-limited imaging possible on large ground-based telescopes, thus opening new fields of discovery. Her work on laser guide stars has resulted in an ongoing revolution in ground-based astronomy. Max led a group that built the AO system and sodium laser guide star for Lick Observatory on Mount Hamilton in California and designed the laser beacon and AO system for the W. M. Keck Observatory in Hawaii in collaboration with Keck Observatory staff. She also was instrumental in creating the newly formed Center for Adaptive Optics headquartered at UCSC.

Max joined the Laboratory in 1974 as part of a new group formed to understand the plasma physics of laser fusion. In the 1980s, she became the founding director of the Institute of Geophysics and Planetary Physics, a position she held for nearly a decade. She also was the first female member of the elite JASON group of scientific advisers to the Department of Defense.

**Edgar A. Leon**, a computer scientist in the Livermore Computing Division, was named a **senior member** of the **Institute of Electrical and Electronics Engineers** (IEEE). Leon has spent his career helping develop increasingly powerful high-performance computing (HPC) systems. He was involved in preparing the Laboratory for the Sequoia supercomputer and is now laying the groundwork for the Sierra supercomputer, scheduled for delivery in 2017. Leon's pioneering contributions include a mechanism to simulate novel computer architectures in large systems and the application of "cache injection" to HPC. His research at Livermore is part of a larger effort to develop and leverage exascale-computing capabilities to ensure the nation's global leadership in HPC. In particular, Leon works on performance and reliability of communication libraries at scale, emerging memory technologies for exascale systems, power-aware computing strategies, and resilience of future systems.

IEEE is the world's largest professional association dedicated to advancing technological innovation and excellence. Only 7 percent of IEEE members attain the level of senior member, which requires 10-plus years of professional experience and significant contributions, achievements, publications, and course development or technical direction in IEEE-designated fields.

## Awards

The Ultrascale Visualization Climate Data Analysis Tools (UV-CDAT) system, developed by Lawrence Livermore and nine partners, has netted the team the **Interagency Partnership Award** from the **Federal Laboratory Consortium for Technology Transfer** (FLC). A nationwide network of federal laboratories, FLC provides a forum to develop strategies and opportunities for linking the laboratory mission technologies and expertise with the marketplace.

UV-CDAT integrates more than 70 disparate scientific software packages and libraries for large-scale data analysis and visualization and serves as a valuable tool for the climate community. The UV-CDAT team consists of Livermore, Lawrence Berkeley, Los Alamos, and Oak Ridge national laboratories; the National Aeronautics and Space Administration's Goddard Space Flight Center; the National Oceanic and Atmospheric Administration's Earth System Research Laboratory; New York University; the University of Utah; Kitware, Inc.; and Tech-X Corporation.

**Natalia Zaitseva**, a Lawrence Livermore physicist, was inducted into the **Alameda County Women's Hall of Fame** in March. One of 12 new inductees, Zaitseva was recognized for her work in science, technology, and engineering.

While working on her Ph.D. at Moscow State University, Zaitseva developed a method for growing extremely large crystals faster than ever before, demonstrating that crystals from solution could be grown 10 to 100 times faster than by traditional methods. She perfected the process after arriving at Livermore in 1993. This work has been important for the National Ignition Facility and has potential applications in national security, energy, and basic research. The Alameda County Women's Hall of Fame was established in October 1993 to recognize outstanding women in the county for their achievements and contributions to the county and its citizens.

**Felicie Albert**, an experimental physicist at Lawrence Livermore, was selected by the **American Physical Society** (APS) as an **Outstanding Referee** for 2015. Outstanding Referees are honored for their exceptional helpfulness in assessing manuscripts for publication in the *Physical Review* journals.

Albert is one of 142 referees being recognized in 2015. This year's selection was made from 30 years of records on more than 65,000 referees who have been called upon to review manuscripts, including more than 37,800 that were submitted in 2014. The basis for selection includes the quality, number, and timeliness of referee reports, without regard for membership in the APS, country of origin, or field of research.

Albert, an expert in ultrafast x-ray sources and laser–plasma interactions, has worked on the Laboratory's laser-Compton light source technology and currently works on the development of betatron x-ray sources for high-energy-density science at the Laboratory's Jupiter Laser Facility and National Ignition Facility (NIF) and SLAC's Linac Coherent Light Source as well as for other NIF and Photon Science Principal Directorate programs.

## Abstract

### Helping Cities Prepare for a Disaster

Federal agencies are working to help cities better prepare for the critical minutes and hours following a disaster, both natural and human-caused. Toward that end, Livermore researchers are using advanced modeling to show that many lives can be saved during incidents that once seemed impossible for which to prepare, in particular for events that can occur without warning. Livermore simulations, shared with federal, state, and local agencies nationwide, are serving as excellent training tools and forming the basis for community-specific emergency response plans. In particular, Livermore researchers are assisting the Federal Emergency Management Agency and other Department of Homeland Security agencies to further the science-based understanding of what to expect from detonation of an improvised nuclear device (IND) or dispersal of a toxic chemical. During such an event, responders would be working with incomplete information, under severe time pressure, and, very likely, in the midst of mass panic and confusion. For example, simulations show how the dense urban landscape can mitigate the effects of an IND as well as provide protection from radioactive fallout. The most important message derived from the advanced models is that many lives can be saved with appropriate planning and preparedness.

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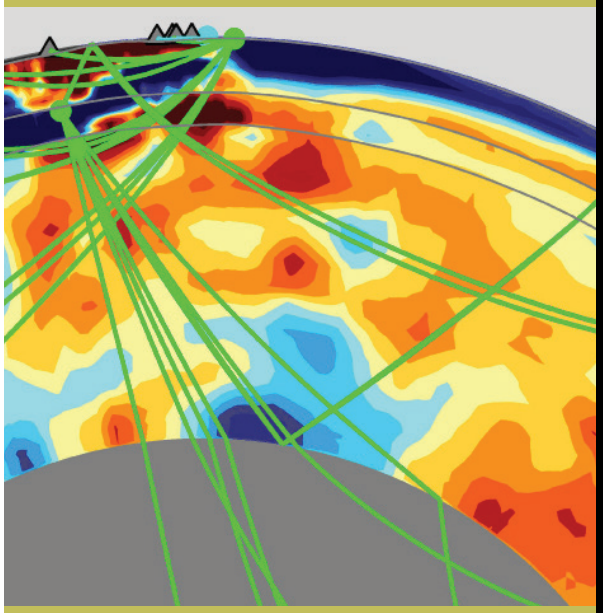
U.S. Government Printing Office: 2015/570-075-10010

# Deciphering Seismic Waves



New technologies are improving the accuracy with which seismic events—including illicit nuclear blasts—are located and characterized.

***Also in June***

*• Livermore scientists and technologies take part in an integrated field exercise in support of the Comprehensive Nuclear-Test-Ban Treaty Organization.*

*• Tying the worlds of electronics and biology together, researchers develop synthetic analogs of biological membrane channels, opening new possibilities for use in synthetic cells, targeted drug delivery, and biosensing.*

*• Livermore-developed lightweight micro- and nanoscale materials for laser experiments and aerospace applications demonstrate superior strength and stiffness.*

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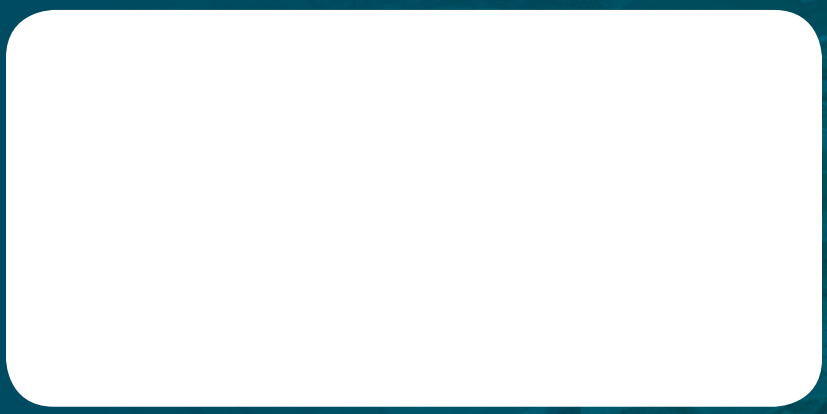

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